DOCUMENT RESUME

ED 247 083 SE 044 673

TITLE	Computational Modeling and Mathematics Applied to the Physical Sciences.
INSTITUTION	National Academy of Sciences - National Research Council, Washington, D.C.
SPONS AGENCY	Department of Energy, Washington, D.C.
PUB DATE	84
CONTRACT	DE-FG1081ER12001
NOTE	105p.
AVAILABLE FROM	Office of Mathematical Sciences, National Research Council, 2101 Constitution Avenue, NW, Washington, DC 20418.
PUB TYPE	Reports - Descriptive (141)
EDRS PRICE	MF01/PC05 Plus Postage.
DESCRIPTORS	*Algorithms; Biological Sciences; Computer Oriented Programs; Engineering; Engineering Education; Higher Education; *Mathematical Applications; *Mathematical Models; *Mathematics; Mathematics Education; *Physical Sciences; Science Education
IDENTIFIERS	*Computational Modeling

ABSTRACT

One aim of this report is to show and emphasize that in the computational approaches to most of today's pressing and challenging scientific and technological problems, the mathematical aspects cannot and should not be considered in isolation. Following an introductory chapter, chapter 2 discusses a number of typical problems leading to computational modeling from the viewpoint of the scientific or engineering discipline in which they arise. Areas considered include: hydrodynamic systems; chemical systems and combustion; plasma physics; particle physics; condensed-matter physics; geophysical applications; meteorology; astrophysics; structural mechanics; nondestructive testing and tomographic reconstruction; mathematical models in the biological sciences; and electronic components. Chapter 3 examines several of the problems from the viewpoint of the computational and mathematical difficulties that arise in connection with them. These difficulties include larger numbers of degrees of freedom, different time or length scales, or singularities of various types. Chapter 4 focuses on the numerical algorithms involved in the computations, such as various discretization methods, continuation approaches, and splitting techniques. Increased support for computational modeling and applied mathematics, computing facilities, and for education and manpower development in these areas is recommended. (JN)

****
* Reproductions supplied by EDRS are the best that can be made *
* from the original document. *
****

NRC NAS NAE IOM

ED247083

U.S. DEPARTMENT OF EDUCATION
NATIONAL INSTITUTE OF EDUCATION
EDUCATIONAL RESOURCES INFORMATION CENTER (ERIC)

☑ This document has been reproduced as received from the person or organization originating it.

☐ Minor changes have been made to improve reproduction quality.

- Points of view or opinions stated in this document do not necessarily represent official NIE position or policy.

Computational Modeling and Mathematics Applied to the Physical Sciences

SE044678

"PERMISSION TO REPRODUCE THIS MATERIAL HAS BEEN GRANTED BY
J. Olson

TO THE EDUCATIONAL RESOURCES INFORMATION CENTER (ERIC)."

Computational Modeling and Mathematics Applied to the Physical Sciences

Committee on the Applications of Mathematics
Office of Mathematical Sciences
Commission on Physical Sciences, Mathematics, and Resources
National Research Council

NATIONAL ACADEMY PRESS
Washington, D.C. 1984

NOTICE: The project that is the subject of this report was approved by the Governing Board of the National Research Council, whose members are drawn from the councils of the National Academy of Sciences, the National Academy of Engineering, and the Institute of Medicine. The members of the committee responsible for the report were chosen for their special competences and with regard for appropriate balance.

This report has been reviewed by a group other than the authors according to procedures approved by a Report Review Committee consisting of members of the National Academy of Sciences, the National Academy of Engineering, and the Institute of Medicine.

The National Research Council was established by the National Academy of Sciences in 1916 to associate the broad community of science and technology with the Academy's purposes of furthering knowledge and of advising the federal government. The Council operates in accordance with general policies determined by the Academy under the authority of its congressional charter of 1863, which establishes the Academy as a private, nonprofit, self-governing membership corporation. The Council has become the principal operating agency of both the National Academy of Sciences and the National Academy of Engineering in the conduct of their services to the government, the public, and the scientific and engineering communities. It is administered jointly by both Academies and the Institute of Medicine. The National Academy of Engineering and the Institute of Medicine were established in 1964 and 1970, respectively, under the charter of the National Academy of Sciences.

This work was sponsored by the U.S. Department of Energy under contract number DE FG1081ER12001.

Available from
Office of Mathematical Sciences
National Research Council
2101 Constitution Avenue, NW
Washington, DC 20418

COMMITTEE ON APPLICATIONS OF MATHEMATICS

WERNER C. RHEINBOLDT, University of Pittsburgh, *Chairman*
JAMES G. GLIMM, New York University
JAMES M. HYMAN, Los Alamos National Laboratory
ROBERT J. KEE, JR., Sandia National Laboratories
JAMES A. KRUMHANSL, Cornell University
JOHN E. OSBORN, University of Maryland
MARTIN H. SCHULTZ, Yale University
IVAR STAKGOLD, University of Delaware

JACOB K. GOLDHABER, *Executive Secretary*

The Committee on Applications of Mathematics is a standing committee of the Commission on Physical Sciences, Mathematics, and Resources of the National Research Council. It is charged with taking all actions deemed appropriate to enhance the effectiveness of mathematics and mathematical statistics in their applications.

COMMISSION ON PHYSICAL SCIENCES, MATHEMATICS, AND RESOURCES

HERBERT FRIEDMAN, National Research Council, *Chairman*
ELKAN R. BLOUT, Harvard Medical School
WILLIAM BROWDER, Princeton University
BERNARD F. BURKE, Massachusetts Institute of Technology
HERMAN CHERNOFF, Massachusetts Institute of Technology
MILDRED S. DRESSELHAUS, Massachusetts Institute of Technology
WALTER R. ECKELMANN, Sohio Petroleum Company
JOSEPH L. FISHER, Office of the Governor, Commonwealth of Virginia
JAMES C. FLETCHER, University of Pittsburgh
WILLIAM A. FOWLER, California Institute of Technology
GERHART FRIEDLANDER, Brookhaven National Laboratory
EDWARD A. FRIEMAN, Science Applications, Inc.
EDWARD D. GOLDBERG, Scripps Institution of Oceanography
CHARLES L. HOSLER, JR., Pennsylvania State University
KONRAD B. KRAUSKOPF, Stanford University
CHARLES J. MANKIN, Oklahoma Geological Survey
WALTER H. MUNK, University of California, San Diego
GEORGE E. PAKE, Xerox Research Center
ROBERT E. SIEVERS, University of Colorado
HOWARD E. SIMMONS, JR., E. I. du Pont de Nemours & Co., Inc.
JOHN D. SPENGLER, Harvard School of Public Health
HATTEN S. YODER, JR., Carnegie Institution of Washington

RAPHAEL G. KASPER, *Executive Director*

CONTENTS

Overview 1
1. Introduction 3
2. Applications 8
    2.1 Hydrodynamic Systems 8
    2.2 Chemical Systems and Combustion 17
    2.3 Plasma Physics 24
    2.4 Particle Physics 26
    2.5 Condensed-Matter Physics 27
    2.6 Geophysical Applications 31
    2.7 Meteorology 33
    2.8 Astrophysical Applications 35
    2.9 Structural Mechanics 37
    2.10 Nondestructive Testing and Tomographic Reconstruction 38
    2.11 Mathematical Models in the Biological Sciences 41
    2.12 Electronic Components 45
3. Computational and Mathematical Difficulties 47
    3.1 Degrees of Freedom 47
    3.2 Different Time and Length Scales 49
    3.3 Singularities in Coefficients, Data, or States 52
    3.4 Boundary Conditions 52
    3.5 Bifurcations and Chaos 54
    3.6 Ill-Posed Inverse Problems 59
    3.7 Effective Media 61
    3.8 Validation, Error Assessments, and Sensitivity Analysis 63
4. Numerical Methods 67
    4.1 Discretization Methods 67
    4.2 Adaptive Grid Methods 72
    4.3 Methods for Solving Discretized Differential Equations 75
    4.4 Continuation and Homotopy Methods 78
    4.5 Optimization Methods 80
    4.6 Graph-Theoretical Methods 81
    4.7 Splitting Methods and Defect Corrections 84
    4.8 Monte Carlo Techniques 85
    4.9 Problem-Dependent Methods 89
    4.10 Computer Software and Hardware 93
Appendix A: Persons Contributing to this Report 96

OVERVIEW

The 1980s are a time of profound challenge to the technological strength of the United States in the economic as well as the military spheres, and our country's performance in research and development in its engineering laboratories will be an important and perhaps determining aspect of our success in meeting this challenge. Advanced engineering development is now based mainly on scientific computation, which in turn relies on mathematical modeling and laboratory experiments. Together they represent one of the areas in which the strength of nations is being tested today.

Mathematics is essential in the development of theoretical and computational models for solving the highly complex problems of engineering and basic science, which encompass a range of scientific difficulties. On one side are questions of computer architecture and the science of algorithms. On the other side is the modeling of chemical and physical processes by means of mathematical equations. The issues are tied together by mathematical theory, which seeks a full understanding of the nonlinear phenomena contained in the equations and implements this understanding through computational methods. This span of scientific activities forms the subject that is known as applied mathematics.

The principal conclusion of this committee is that computational modeling, which is a high-leverage element of our nation's scientific and technological effort, requires increased emphasis and support. The conclusion is documented by an examination of typical application areas, which reveals the pervasive difficulties that accompany computation of realistic problems and leads one to consider both what computers can do and what they cannot currently do but might eventually be capable of doing. As illustration, we examine several deep theoretical problems, including turbulence and combustion. At the frontiers of attack on these problems we discover the limitations imposed by our current understanding of model formulation and computational capability. We examine modeling problems and algorithms adapted both to specific features of the desired solution and to the computer architecture. We also examine computer architecture and component design and manufacture as a mathematical modeling problem.

The Committee recommends increased support for

1. Research in computational modeling and applied mathematics,

2. Computing facilities dedicated to this area,

3. Education and manpower development in computational and applied mathematics.

These recommended increases include financial support from government and industry as well as institutional support from universities.

1. INTRODUCTION

The extensive use of computers in advanced development work began during World War II, and today computing is a vital component of science, engineering, and modern technology. Most advanced technological development, from aircraft design to automobiles to petroleum to satellites now follows this pattern of reliance on the computer. Moreover, the needs of national defense have posed scientific and engineering design problems as difficult as any ever encountered. Numerical computation and applied mathematics have played an essential role in dealing with such problems. In fact, numerical fluid dynamics was born during the 1940s for the purpose of assisting in the design of nuclear weapons, combat aircraft, and conventional ordnance and is now applied widely by industry.

Most problems of engineering or scientific interest are too complex to be modeled and computed exactly. Instead one considers a series of approximate models and computations, each of which illuminates a different aspect or idealized portion of the overall problem. When used by a skilled engineer or scientist, these mathematical models greatly enhance the judgment that goes into design decisions and reduce the amount of expensive laboratory and field testing required. These advantages account for the widespread use of these models.

More specifically, mathematical models are used in engineering design problems in the following modes:

1. To provide the first test of a new design idea. Beyond common sense and simple hand calculations, the computer model is usually the cheapest and fastest test of an idea. This test is applied before deciding whether to conduct a series of experiments or to build a prototype.

2. To reduce the time and cost associated with laboratory and field tests. Usually engineering problems contain several critical design parameters that will have involved a certain amount of trial and error in the search for the optimum choice. The computer is used qualitatively (Will an increase in parameter X improve or degrade performance – or performance parameter Y?) and quantitatively (Which values of design parameters $X_1, \ldots, X_n$ will optimize performance?).

3. To assist in laboratory or field tests that determine model parameters and equations. Often the model parameters are measured

only indirectly. Thus, a computer model of the laboratory apparatus may be needed to extract the desired information from the observed data. Usually these models are simpler than the complex engineering models, and their defining equations can be solved with greater precision and fewer approximations.

4. To replace laboratory or field tests. Sometimes tests are impossible or impracticable. For example, measurement of chemical reaction rates at extreme conditions of pressure and temperature is very difficult, and accumulated experience through trial and error is not adequate for solving the problem of landing the Space Shuttle, for reasons of human safety as well as cost.

5. To improve the education and judgment of engineers and scientists using the models. The mathematical models and computer solutions provide a vast increase in the quality and caliber of the data. Thus while the laboratory measurement may produce some overall quantity (e.g., total flow in and out), the computer model might yield detailed velocities and concentrations at each point of the flow field. Because the equations are nonlinear, it is difficult to foresee all the relevant phenomena, much less to understand their relative importance. Thus the model becomes for users an experimental tool that allows them to understand a problem at a level of detail that cannot be achieved by other means.

In summary, mathematical and computer models are used because they are faster, cheaper, and more effective.

However, models have limitations. There are limitations in the validity of the equations used, in the adequacy of the solution algorithm, and in the size and speed of the computer. Also, the cost, accessibility, and reliability of computer software and, sometimes, the cost of the computation itself can be limiting factors. These limitations in some sense define the frontiers of science, but more specifically they define the frontiers of applied mathematical science.

Problems of realistic interest typically involve the study of diverse physical phenomena on many scales of length in fully three-dimensional settings. Though essential, experimental science in these contexts is expensive and difficult. The design of modern strategic weapons systems epitomizes these characteristics. For example, in the design of a TRIDENT submarine, the architecture of the vessel, the design of the missile, and the design of the nuclear warhead all need to be modeled and integrated, which requires many thousands of hours of computer time and stretches available computing power and modeling techniques to their limits.

Generally, design and evaluation of new kinds of defense systems, such as remotely controlled or robotic vehicles, will require analysis of entirely novel systems, using parallel computer architectures among other things. The needs of industry for technological advances are similar and are dominated by such basic concerns as pollution, depletion of resources, energy conservation, and efficient use of manpower. It seems safe to say that defense and industrial needs will continue to lead numerical computation and applied mathematics into new and challenging regimes.

Depending on the complexity of the problem and the magnitude of the effort expended, models range from excellent to merely suggestive in their quality and usefulness. In all cases, improvement of computer modeling is one of the most promising avenues to improved technological performance by our nation.

As one of the aims of this report, the Committee wants to show and emphasize that in the computational approaches to most of today's pressing and challenging scientific and technological problems the mathematical aspects cannot and should not be considered in isolation. There is a unity among the various steps of the overall modeling process from the formulation of the physical problem to the construction of appropriate mathematical models, the design of suitable numerical methods, their computational implementation, and, last but not least, the validation and interpretation of the computed results. In particular, the Committee wants to illustrate that the steps are more often than not deeply interconnected and that the computational process may indeed be part of the model construction. At the same time, there are problem areas, such as turbulence, where current theoretical research may promise a deeper insight into an important physical phenomenon.

In line with these aims, the report uses a "matrix approach" that views the same problem from three different standpoints. In Chapter 2, the traditional approach is taken of discussing a number of typical problems leading to computational modeling from the viewpoint of the scientific or engineering discipline in which they arise. Then in Chapter 3 certain of these problems are touched on again, this time from the viewpoint of the computational and mathematical difficulties that arise in connection with them. For example, these difficulties may involve large numbers of degrees of freedom, different scales of time and length, or singularities of various types. In Chapter 4 the viewpoint becomes that of the numerical algorithms involved in the computations, such as various discretization methods, continuation approaches, and splitting techniques.

Of necessity, many topics have been left out. The list of applications, for example, is by no means complete, and, in fact, entire areas such as reactor safety and reactor physics are not mentioned at all. Neither did the Committee attempt to address all computational and mathematical difficulties nor all variations of numerical algorithms. The choice of topics was motivated in part by energy-related considerations, the expertise and interests of the Committee and its advisers, and the report's broad purpose, whose achievement would be hindered by any attempt to be encyclopedic. For the same reason, the report is not intended to be a technical summary, and this is also reflected in the fact that no attempt was made to reference the relevant literature. The report is mainly addressed to scientifically literate readers who know how to consult the literature when necesary.

The Committee obtained advice and technical support from many colleagues across the country and from abroad. A list of names of all those who helped in this work is given in Appendix A, and the Committee is extremely grateful for all the often extensive documentations, special write-ups. and other comments that we received. The report is the result of a study begun by the Committee in 1981 on computational mathematical modeling and mathematics applied to the physical sciences with particular reference to the needs of the Department of Energy (DOE). The preparation of the report was supported by the Applied Mathematical Sciences Research Program of the Office of Basic Energy Sciences of DOE, and the Committee also expresses its thanks and appreciation for this support.

As stressed in the Overview, the Committee found that improvement of the mathematical and computer modeling of scientific problems is an important priority for our nation. The challenge is broad, and there are no simple remedies for current shortcomings. Accordingly, the Committee recommends the following:

1. Increased research support for computational modeling and applied mathematics

The technological challenges of the coming decades will impose new tests of our abilities in computational and applied mathematics, and meeting the tests will require increased research effort. As illustrated in this report, the challenges are typically multidisciplinary in nature with applied mathematics and modeling often in a central position.

Hence, to support research in this area, multidisciplinary teams of adequate size to make progress on these complex problems should be encouraged; and organizational means should be devised to facilitate their establishment, continuity, and success.

2. Increased support for computing facilities dedicated to computational modeling and applied mathematics

Ready access to modern computing systems is essential. Lack of equipment is the critical factor most strongly limiting academic research in computational mathematics. There is need both for conveniently usable local equipment and for access to large-scale computers. Local facilities are necessary for entire problems of modest size and for such tasks as code development, interactive debugging, test runs, and graphical analysis. Large-scale computing is essential because of the size of many typical problems as documented in this report. In this connection, the Committee strongly endorses the findings and recommendations in the recent *Report of the Panel on Large-Scale Computing in Science and Engineering*, Peter D. Lax, Chairman, National Science Foundation, December 26, 1982.

3. Increased support for education and manpower development in computational and applied mathematics

Today there are unmet manpower needs in computational and applied mathematics, as discussed, for example, in *Science and Engineering Education for the 80s and Beyond*, a National Science Foundation report, October 1980. These needs are found in industry, government laboratories, and academic institutions. The critical challenges in this area call for a focus on quality. Specifically, the complex interdisciplinary nature of the problems poses special educational challenges for students and young researchers, and graduate and postdoctoral fellowship support for participation in multidisciplinary teams of the type discussed above would also be helpful.

A valuable aspect of such multidisciplinary education is the interaction it creates between applied mathematicians and other applied scientists in universities, government, and industry.

2. APPLICATIONS

2.1 HYDRODYNAMIC SYSTEMS

Hydrodynamic processes touch nearly every aspect of our lives. In a report even many times larger than the present one, we could not possibly discuss all hydrodynamics applications. Therefore, we have chosen a few, with the hope that they will serve to illustrate the importance of hydrodynamic models and to point out some of the problems that occur in developing the models.

A large fraction of the current research in computational modeling is done with hydrodynamics applications in mind. The great variety of responses that we received to our requests for material for this report attest to the diversity of these applications. Among them were applications having to do with aircraft and wing design, both at subsonic and supersonic speeds; global weather prediction and local phenomena such as tornadoes; water waves and ship hull design; piping networks, such as in nuclear reactor or power plant design; geologic phenomena, such as glacier flow or convection in the Earth's mantle; biological flows, such as the flow of blood in the heart; and chemically reacting flow, such as combustion.

The general system of equations governing hydrodynamics are called the Navier-Stokes equations. They are a statement of mass and momentum conservation, the momentum equation being a formulation of Newton's second law, $F = ma$. The Navier-Stokes equations were first developed in France by Navier in the early 1800s. They represented an improvement over the Euler equations that were first derived in 1755, in that the Navier-Stokes equations included viscous effects that were absent in the Euler equations. However, it was not until 1904, when Prandtl developed the boundary-layer approximations, that predictions of practical viscous flows could be made. Practical solution of the full Navier-Stokes equations had to await the development of modern high-speed computers beginning in the 1940s.

Why are equations that have been known for over 100 years so hard to solve? The answer lies largely in their inherent nonlinear characteristics. Immediately upon looking at the equations one sees that the convective transport terms (the acceleration in $F = ma$) involve velocity times its gradient. This nonlinearity is always present, and it is responsible for the existence of complex phenomena such as shock waves and turbulence. In principle the Navier-Stokes equations alone provide a description of turbulence; however, one would have to resolve such small length scales in their solution that this approach is not of practical importance. Therefore, a great many approaches to approximating turbulence effects are being pursued. Typically, these models introduce further nonlinearities into the system.

Other problems that arise in the solution of hydrodynamic problems are related to the disparate time and length scales that must be resolved. In particular, convective transport is characterized by the fluid velocity, whereas pressure waves travel at the sound speed–typically orders of magnitude faster than fluid speeds. At the same time the effects of diffusive processes (e.g., shearing stresses) are felt instantaneously throughout the flow. In some cases the fluid can react chemically. In those cases, the reaction rates display a strong nonlinear dependence on the fluid temperature. This introduces yet more characteristic scales into the models.

Depending on characteristic parameters such as the Reynolds number, the solutions to the Navier-Stokes equations either can be smooth and steady or they can exhibit regular oscillations. Or they can be completely chaotic. It is clear that depending on the regime the appropriate solution procedures could be quite different.

Finally a word about boundary conditions. In some problems the flow is enclosed, and hence boundary conditions are applied at the boundaries of the enclosure (e.g., an automobile engine cylinder), which can often have a complex shape. In other cases, such as an aircraft wing, the flow is effectively unbounded, and the boundary condition should be applied at "infinity" (see Section 3.4). Some modeling problems arise in approximating infinity by some finite boundary. In still other problems, such as the flow of blood in a heart, the boundary is both complex in shape and deforms depending on the forces exerted on it by the fluid. Modeling such a problem is clearly a challenge.

2.1.1 Wings, Wind Tunnels, and Computers

The economics of the energy shortage implies that planes will fly at speeds close to but less than the speed of sound. At such speeds there is a "supersonic bubble" over the wing, where the local velocity of the air relative to the wing is greater than the speed of sound. In this case the presence of shock waves is typical and undesirable. They are undesirable

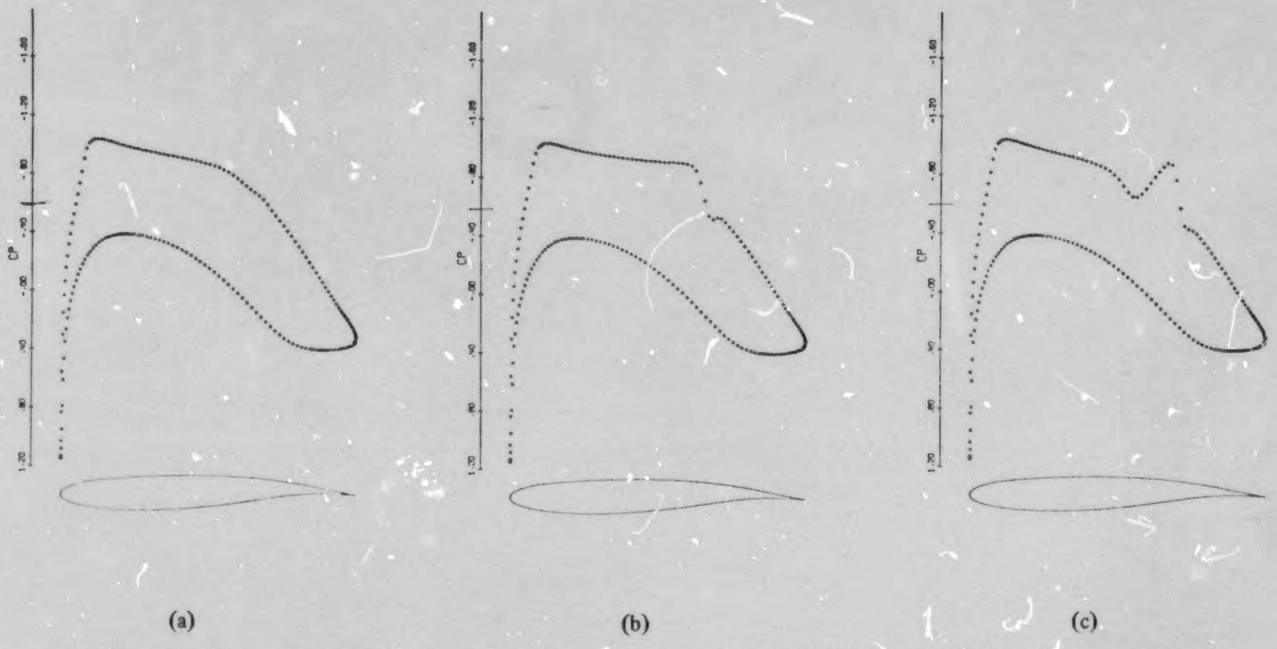


FIGURE 2.1 Distribution of velocity (normalized) on surface of a Korn supercritical airfoil at Mach numbers 0.750, 0.752, and 0.748. The long bar at left is the transition value. [From C. S. Morawetz, The mathematical approach to the sonic barrier, *Bull. Am. Math. Soc.* **6**, 127-143 (1982).]

because the drag can be computed as being proportional to the third power of the shock strength. The goal of efficient wing design is to produce wing shapes with no shocks or only weak shocks in this transonic region. A general mathematical theory shows that shockless wing foils exist for given transonic cruising speeds. However, the problem of finding such wing shapes is both overdetermined and extremely sensitive to small changes in the data, i.e., "ill-posed" (see Section 3.6). The solution to such ill-posed problems is still valid from an engineering point of view because operation at neighboring off-design conditions will produce only weak shocks and small drag, see Fig. 2.1.

Using computer algorithms created by applied mathematicians, it is now possible to solve both the inverse problem (design) and the forward problem (of determining the flow field for a given wing shape and velocity) with sufficient accuracy that the use of costly wind-tunnel experiments can be greatly reduced. This accomplishment is a striking success of recent applied mathematics.

The theoretical areas that have contributed to this study include the theory of nonlinear elliptic equations, complex function theory, and mixed problems, for which a prototype is the Tricomi equation,

$$y\frac{\partial^2\phi}{\partial x^2}+\frac{\partial^2\phi}{\partial y^2}=0$$

which is elliptic for $y > 0$ and hyperbolic for $y<0$. The elliptic region corresponds to the subsonic region, and the hyperbolic region to the supersonic "bubble." In a numerical method for the design problem, an analytic continuation makes the elliptic region hyperbolic. The resulting equation is solved by the method of characteristics, and then the analytic continuation back to real values of space is performed numerically.

2.1.2 Chaos, Turbulence, and Droplets

Turbulence produces a boundary layer along the trailing edge of an aircraft wing. The boundary layer degrades the wing performance and thus is an important part of the design problem. The flow behind the trailing edge of a wing contains a vortex sheet, and the roll-up of this vortex sheet produces turbulence that constitutes a safety hazard for small aircraft flying in the wake of a jumbo jet. The axis of the vortex roll-up is perpendicular to the wing, and so the roll-up is intrinsically three dimensional. In the simpler case of two-dimensional flow the vortex sheet is a line or curve in the plane, emanating from the trailing edge of the wing foil. In regions in which the line is stretching, it is geometrically stable. In regions in which it is contracting, it is unstable. Instead of contracting, it forms a spiral vortex structure and hence is stable.

The two-phase flow of water and steam in a cooling pipe, or of oil and gas in an oil-reservoir production well, is also a problem in which the geometrical instabilities of large-scale fluid motion are important. Here an internal movable boundary separates regions of different material properties. In some cases (a heavy fluid, e.g., water, falling into a light fluid, e.g., air), the material interface is unstable against formation of fingers. There is continuation of the nonlinear instabilities leading to pinchoff of droplets and a chaotic regime (mist) that can be analyzed on various length scales, as discussed below in the case of turbulence.

During the combustion stroke of an automobile engine, the flame is quenched when it reaches the cold cylinder walls, and incompletely burned fuel present in the combustion chamber at this time contributes to pollution and to a loss of fuel efficiency. The rate of advance of the flame from the spark plug to the cylinder walls is governed by the laminar flame speed and the rate of turbulent mixing. Of these two effects, the second is more important. The turbulent mixing is produced by vortices that detach from the turbulent boundary layer at the wall during the intake and compression strokes (see Fig. 2.2). Thus, an accurate modeling of this problem requires an ability to treat a number of fluid singularities: flame fronts, vortices, turbulence, boundary layers, and boundary-layer separation.

The examples above show that singularities in fluid flow may be geometrically unstable. When this instability occurs in a regime governed by the scale-invariant Euler equations, the phenomenon is repeated on all length scales and leads to chaotic solutions. Turbulence, vortex roll-up, convection fingering, and droplet formation are examples of this phenomenon, which we now discuss from a general point of view.

The Euler equations of fluid dynamics allow intrinsic singularities, namely vortices, boundary and shear discontinuity layers, contact or material interface discontinuities, and shock waves (Fig. 2.3 shows a computation of the stretching of a vortex tube in a periodic inviscid flow). Depending on the problem, special discontinuities such as flame fronts or chemical reaction fronts (for fluid dynamics with chemistry) may occur. Within the singularity, the Euler equations fail to be a correct description of nature, and corrections (either parabolic effects or perhaps a more complicated Euler equation with more state variables) may be required. As an example, consider a shear layer (i.e., a jump discontinuity in the tangential velocity component). Taking the curl of the Navier-Stokes equations, we obtain for

$$\omega = \nabla \times v = \text{vorticity}$$

the equation

$$\frac{\partial \omega}{\partial t} + (v \cdot \nabla)\omega - (\omega \cdot \nabla)v = \nu \Delta \omega$$

where ν is the kinematic viscosity. To understand the significance of this equation, we specialize to two dimensions. Then ω is a vector in the z direction, $(\omega \cdot \nabla)v$, and

$$\frac{d}{dt} + (v \cdot \nabla)$$

is the total, or Lagrangian time derivative, so that the Navier-Stokes equation says that vorticity moves by passive transport plus diffusion. The extra term, $(\omega \cdot \nabla)v$ above, induces vortex production as a result of the stretching of vortex lines in three dimensions and is important for considerations of geometrical stability as discussed below. In summary, the diffusion term $\nu \Delta v$ of the Navier-Stokes equation is responsible for the vorticity leaving a boundary or internal shear layer and diffusing into the rest of the flow. Without viscosity there is no mechanism for vorticity to enter (an initially irrotational) flow region. The Prandtl boundary-layer

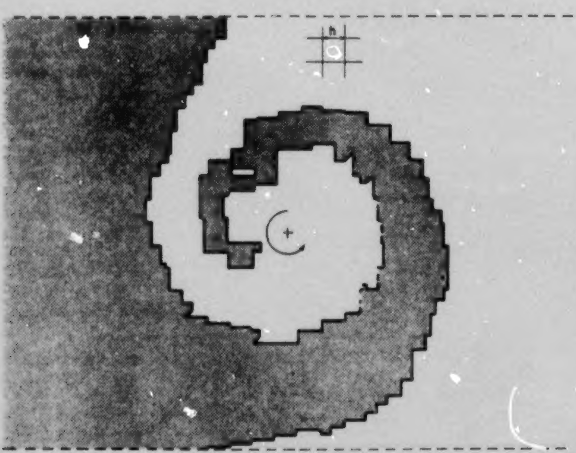


FIGURE 2.2 Stretching of a flame by a vortical structure. Such stretching is important for the efficient operation of engines; it enhances burning by increasing the area of the flame. [From A. J. Chorin, Flame advection and propagation algorithms, *J. Comput. Phys.* **35**, 1-11 (1980).]

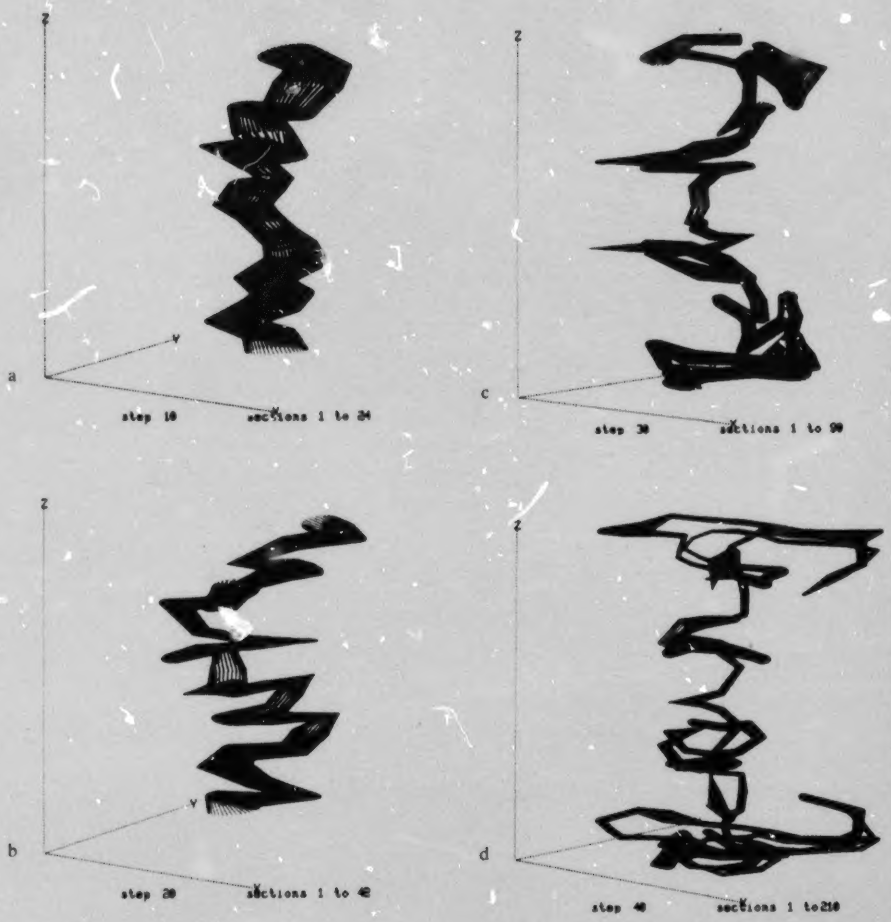


FIGURE 2.3 Successive stages in the stretching of a vortex tube in an inviscid periodic flow. Vortex stretching is the mechanism by which energy in a turbulent flow is transferred to ever smaller scales where it is eventually dissipated. a, step 10, time = 0.65; b, step 20, time = 0.88; c, step 30, time = 1.04; d, step 40, time = 1.21. [From A. J. Chorin, The evolution of a turbulent vortex, *Commun. Math. Phys.* **83**, 526-527 (1982).]

equations are a special version of the Navier-Stokes equations (scaled in the normal direction, so that diffusion occurs only normal to the boundary).

Often the fluid singularities are geometrically unstable. They may bifurcate in a predictable fashion, developing "rolls" (Couette flow) or "cells" (Bénard flow), or they may become irregular and highly convoluted with a tendency toward chaos, known as turbulence. There is no scientific reason to question the validity of the Navier-Stokes equation as a microscopic description of physics even into the turbulent regime. However, its usefulness as a description of large-scale fluid motions in the turbulent region can be questioned, and some other description of fluid flow, such as a random ensemble of interacting vortices, could be more effective.

There are three energy or length scales in which quite distinct characteristic phenomena dominate. The smallest length scale is that on which energy dissipation dominates. On this length scale, the Navier-Stokes equations are the correct equations. The viscosity is large, causing velocity fluctuations to be rapidly smoothed and solutions to be (locally) "laminar." Since smoothness of solutions is a local property, we may conjecture that all solutions of the Navier-Stokes equations should be smooth for all time. This conjecture is the major unsolved problem of the energy dissipation range. It is known that solutions with smooth data will remain smooth for a short time, and solutions with smooth and small data will remain smooth for all time. Both statements exclude turbulent regimes.

For weak solutions, Leray showed that the set of times t for which $v(x,t)$ fails to be smooth is a set of measure zero. Recently considerable progress has been made in restricting the possible singularities of the Navier-Stokes equations.

For longer length scales, viscous effects do not play a major role and the fluid flow can be described by Euler equations. However, this simplification gives rise to problems. The problems are not merely technical but reflect the intrinsically complex phenomenology of fluid dynamics. The Euler equations are scale-invariant. Thus if $v = v(x,t)$ is a solution, so is $v = v(\alpha x, \alpha t)$. The inertial range is the set of length scales dominated by scale-invariant, universal physics. Whatever phenomena can occur (e.g., vortices) will be repeated on all length scales in the inertial range. The inertial range is limited at the smaller end by viscous dissipation. At the larger end, it is limited by the special boundary and initial conditions imposed on the flow, which result in special (nonuniversal) flow behavior.

The inertial region is dominated by scale-invariant behavior. There is a flow of energy from large-scale motions to smaller ones (the "energy cascade"). This cascade seems plausible on physical grounds as a type of third law of thermodynamics but does not have a rigorous mathematical status. It can be explained as a consequence of the geometrical instability of vortex lines and shear layers. As these go unstable, they generate (smaller) new vortices and vorticity.

The energy cascade leads to a dimensional analysis of characteristic exponents and to the Kolmogoroff 5/3 power law

$$E(k) \sim k^{-5/3}$$

for the energy distribution as a function of wave number k. A discussion of the experimental data in connection with the Kolmogoroff theory has the vortices, which occur on all length scales in the inertial range, as filling space. Actually, it may be better to assume the contrary: vortices of a given size fill only a small part of space. Then the smaller vortices, which are driven by the larger ones, will occur only within the region of these larger vortices, and in fact only within a small part of this region. This is the notion of intermittency. It leads to the idea of a singular set for solutions of the Euler equations, which is a Cantor set of fractional dimension less than 3.

Intermittency leads to modifications in the Kolmogoroff exponent and to a renormalization group type picture of turbulence. Numerical calculations to determine intermittency and energy cascade exponents have been performed. The calculations start by tracking vortex lines in a fluid flow and proceed through a sequence or renormalization group length scale transformations to focus on the singular Cantor set within the solution.

In most problems, the inertial region contains lengths too small to be used directly in a fluid calculation. Its importance lies in its role of fixing parameters such as an effective or eddy viscosity, which are then used to determine the large-scale motion of the fluid. The inertial region is not particularly well understood from either the theoretical or numerical point of view.

The large-scale fluid motions are produced directly by the initial and boundary conditions imposed on the flow. These motions are strongly problem dependent. Numerical calculations and experiment are important tools in their study as is the detailed analysis of simplified and idealized flow configurations. An important theoretical question is the evolution of initially unstable flow configurations. This question arises in connection with the onset of turbulence and in connection with the energy cascade, where large-scale vortices excite and drive small-scale ones.

In some problems (supercritical turbulence), the instability in an initially laminar flow is nonturbulent but arises from the bifurcation of a fixed point. Further bifurcations lead to higher-dimensional tori, and a general theory explains that generically the flow on the (sufficiently high-dimensional) torus has a strange attractor as its limit set and that this strange attractor is chaotic in nature. This picture has been analyzed in the context of the Lorentz flow, which is the truncation of the Navier-Stokes equations to include only a small number of modes. The strange attractors found there have a Cantor-like structure. An example of supercritical turbulence is Couette flow.

Subcritical turbulence occurs when the finite (noninfinitesimal) perturbation is less stable than the infinitesimal one. Then turbulence occurs below the critical Reynolds numbers at which the linear theory shows instability and may go directly to turbulent behavior without a discrete sequence of nonturbulent bifurcations starting with laminar flow.

2.2 CHEMICAL SYSTEMS AND COMBUSTION

From the invention and manufacture of an enormous range of synthetic materials (e.g., plastics) to the refining and burning of fossil fuels, chemistry and chemical processes affect nearly every phase of our lives. Naturally it is important to understand and control, as fully as possible, many of these complex chemical processes. For example, we seek to find new and better materials, to reduce costs, and to generate energy more efficiently and with less pollution. Applied mathematics and computational modeling continue to play a valuable role in meeting these goals.

One of the oldest chemical processes harnessed by man is combustion. The successful modeling of combustion provides an extraordinarily rich source of challenges for the computational mathematician. Frequently, combustion models have to incorporate all the difficulties of complicated fluid mechanics coupled with complex chemical kinetics. The challenges include developing algorithms to ensure accuracy and to reduce computer time and storage. The modeler also seeks appropriate simplifications that take advantage of any special attributes of the governing physics in order to gain more efficient computation. Since combustion contains a wide range of chemical processes, we use it here as an example to illustrate points of mathematical interest in general chemical systems.

Even within the topic of combustion there is an enormous diversity of applications. The first topic that probably comes to mind is the modeling of internal combustion engines, and this is an important application. Modeling is a part of ongoing research to design new types of engines (e.g., direct injected stratified charge), to improve fuel economy, to utilize alternate fuels (e.g., alcohols), and to reduce pollutant formation. Similarly, research for other combustors such as gas turbines or power-plant boilers benefit from computational models. Still there are many other important combustion problems aside from power generation. For example, the field of fire research is devoted to problems such as how fires spread in buildings and the behavior of various fire-retardant materials. An important current topic in reactor safety is the characterization of hydrogen-air fires such as occurred in the Three Mile Island accident. Another public safety question deals with the problems of fire and explosion associated with a liquid-natural-gas tanker accident. Problems of burning coal and coal gasification are also topics of great current interest.

Perhaps the simplest chemical process from a physical viewpoint is chemical equilibrium. At equilibrium all chemical reactions are assumed to have gone to completion, and the species concentrations are such that the mixture is in a minimum free-energy state. The mathematical computation of the chemical equilibrium state is posed as a constrained minimization problem. In combustion the equilibrium composition corresponds to the products of combustion long after the combustion is complete. Physically, the next step in complication comes with the inclusion of finite-rate chemical reactions. Here the mathematical problem is one of solving systems of stiff ordinary differential equations (see Section 3.2 for a discussion of stiffness). Models of shock tubes or flow reactors, which are used frequently to probe fundamental questions in chemical reaction kinetics, fall into this class of problems. The physical situation is complicated further by the inclusion of fluid motion and heat and mass transport. In this case the mathematical problem is one of solving systems of parabolic or elliptic partial differential equations.

Consider the internal combustion engine as an example. What are the things that we might hope to learn from modeling? Ultimately, we hope to influence geometrical considerations such as combustion chamber shape and component placement (e.g., valves spark plugs, fuel injectors). We also hope to provide a fundamental understanding, on the molecular level, about how fuels are oxidized and how pollutants are formed. With such understanding we can suggest ways to alter the combustion process to advantage. In the past only power and size were important considerations, and engine optimization could proceed mostly experimentally. Now, however, there are too many parameters to optimize simultaneously, and computational modeling is increasingly important.

Because of limitations in available computational resources, two tacks are taken in engine modeling. One is to consider mostly hydrodynamic effects. Here the modeling of boundary shapes and component placement is of primary importance (e.g., How should the piston face be shaped, and where should the spark plug be placed?). Complex domains and two- and three-dimensional effects are important. The models must incorporate

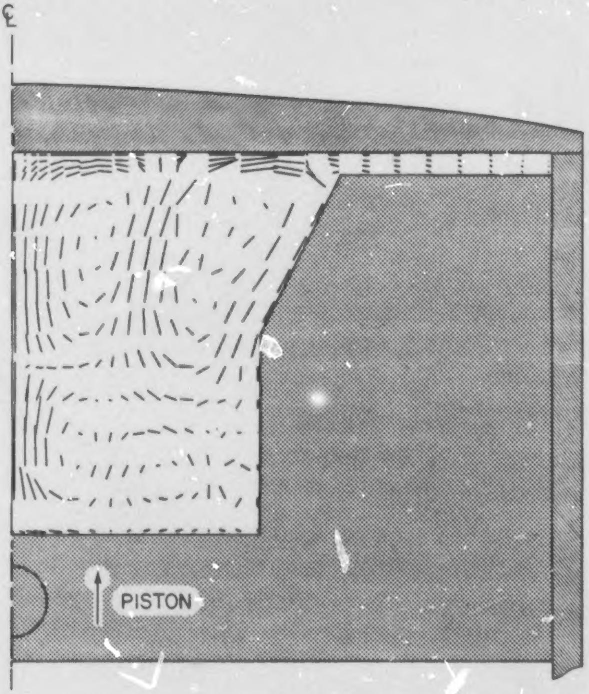


FIGURE 2.4 Velocity vectors computed in a direct-injection, stratified-charge engine at a position near top dead center. The combustion takes place in a swirling environment in a cup-like region machined into the piston. Several vortices are seen to develop in the cup. [From T. D. Butler, L. D. Cloutman, J. K. Dukowicz, and J. D. Ramshaw, Multidimensional numerical simulation of reactive flow in internal combustion engines, *Prog. Energy Combust. Sci.* 7, 293 (1981).]

turbulent hydrodynamic effects and sometimes phase-change processes, such as fuel spray injections. The chemistry is usually simplified in these models because it is not feasible to consider both complex chemical kinetics and hydrodynamics on current computers. Figure 2.4 shows the velocity vectors that result from a two-dimensional simulation of a direct injected stratified charge engine. This is a new engine concept that is being studied in a U.S. Department of Energy-sponsored cooperative program including General Motors Research Laboratories, Princeton University, and three National Laboratories.

In addition to the hydrodynamic aspects of engine combustion, there are important unanswered questions about the chemistry. Therefore, the second tack is to consider simplified hydrodynamic situations, such as laminar flames, and treat the chemical kinetics in great detail. These models address issues such as ignition phenomena and pollutant formation. Figure 2.5 shows some species profiles computed in an atmospheric pressure acetylene-oxygen premixed flame (acetylene is an important reactant in soot formation). This model used 30 chemical species and 103 reactions. The results were computed using an adaptive mesh placement strategy, and they resolve detailed structure within the flame. Note that the flame is very "thin" – its thickness is on the order of one millimeter, while combustion chamber dimensions are on the order of tens of centimeters.

An interesting aside is to note that these two approaches to combustion modeling match corresponding approaches to experimental investigation. That is to say, it is usually not possible to measure or compute minor species concentrations in complex turbulent flows, whereas it is possible to do so in laboratory flames.

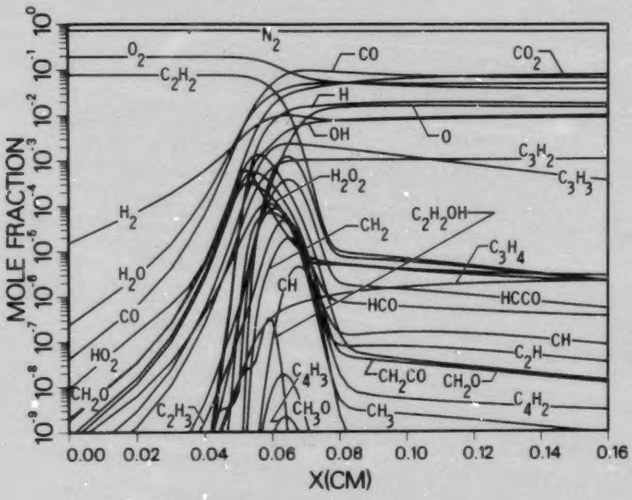


FIGURE 2.5 Species mole fraction profiles showing the internal structure of an atmospheric-pressure stoichiometric acetylene-air flame. [From J. A. Miller and R. J. Kee, Sandia National Laboratories.]

The inherently disparate time scales of chemical reactions, in other words their stiffness, contribute to the numerical difficulty of solving combustion models (see Section 3.2). The inherently disparate time and length scales for fluid transport, heat transfer, and chemical reaction are responsible for the presence of steep fronts in the solutions. Also, there are many degrees of freedom in the system of equations. The number of governing partial differential equations is large because a transport equation must be included for each species involved in the chemical reaction set. A system of 30 to 50 species, involving 100 or more chemical reactions is typical even for fuels as simple as methane. Also, for practical combustors, the model must ultimately include complex three-dimensional geometries. Because complete models of real combustors are too large for present computers, an important challenge is to simplify the models (including the physical assumptions) to a tractable level. In addition to these problems, there are potential difficulties related to scaling. The temperatures are on the order of 10^3 K, while some species can have important effects even when their mass fractions are as low as 10^{-10}. Moreover, before the computation, the peak mass fractions of the various species are usually known only to within several orders of magnitude.

Many of the challenges of combustion modeling have been met by the numerical-analysis community; however, many more await resolution. For example, for systems of ordinary differential equations we understand how to treat the stiffness that results from the complex chemical kinetics by using stable implicit methods. However, for systems of partial differential equations the application of these methods leaves many open questions about how to treat the linear algebra and how to compute the error estimates. Operator splitting methods are important in rendering the linear algebra tractable for large problems. Stiffness also occurs in low-Mach-number flows due to very high velocity, but low-amplitude, pressure waves. Usually, we do not care about the details of these waves, but they can unreasonably limit the size of the time step in explicit methods. Subcycling methods, rather than implicit methods, are sometimes used to alleviate this problem. Subcycling is a form of operator splitting (see Section 4.7) in which the invicid hydrodynamic equations are solved with small time steps, while the viscous parts of the equations and the energy and mass transport equations are solved using a much larger time step.

Another particularly important topic in combustion models concerns the adequate resolution of localized behavior such as flame fronts. One line of research considers adaptive meshing strategies in which a spatial mesh network is adjusted dynamically so as to capture the local behavior accurately. Other work considers front-tracking methods, where the flame is treated as a local discontinuity and conservation equations connect both sides of the front and predict its movement.

Combustion models must account also for fluid turbulence, an area where even the underlying physics is not well understood. Here, computational models such as the random vortex method are proving valuable in simulating turbulence effects, especially in the investigation of large-scale turbulent eddies, the so-called coherent structures. We classify these methods as "problem-dependent methods" because the physics and the numerical model depend heavily on each other (see Section 4.9). Recently, the random vortex method has been combined with a flame propagation algorithm so that combustion events can be modeled. Figure 2.6 is a sequence of computer plots that shows the vortex velocity fields and flame fronts as computed from a model of turbulent combustion behind a step.

2.2.1 Asymptotic Analysis

We mention here that applied analysis (in concert with computation) is valuable for many problems in combustion. Asymptotic methods, for example, can actually take advantage of phenomena such as steep fronts. They can thus be used to provide insights and to suggest approximations that help to reduce the complexity of the numerical models and thus render them more tractable. An important aspect of the asymptotic analysis is the possibility of considering the dynamical stability of flames. Such work may lead to fundamental understanding of such phenomena as the onset of turbulence.

Asymptotic methods exploit the fact that the overall activation energy of the chemical reaction is typically large, a well-known consequence of which is that flame fronts are very thin. That is, chemical reaction is only important in a thin region where the temperature first approaches its burned value. On the unburned side of this region, chemical reaction is negligible because the temperature is too low, and on the burned side, it is negligible because the reaction has essentially gone to completion, depleting the unburned fuel. Mathematically speaking, this thin chemically reactive region may be thought of as an internal boundary layer, separating the unburned and burned gases. In the limit of asymptotically large activation energy, the boundary layer is infinitely thin, and we may use asymptotic matching principles to connect, or match, the solutions inside and outside the boundary layer. The result is a flame sheet model in which the solutions on either side of the sheet are connected by nonlinear jump conditions that depend on local conditions at the front. Though the resulting problem is still nonlinear, it represents a significant simplification over the original problem with Arrhenius kinetics and is in fact equivalent to the original problem in the asymptotic limit of infinitely large activation energy.

The first studies using large activation energy asymptotics began to appear about a dozen years ago and were noteworthy for providing for the first time analytical flame speed formulas for a steadily propagating planar flame. The most significant results to come out of this approach to date are the prediction of instability and bifurcation phenomena, which describe cellular and pulsating modes of flame propagation. These more complex solutions branch, or bifurcate, from the basic solution (in this case, a

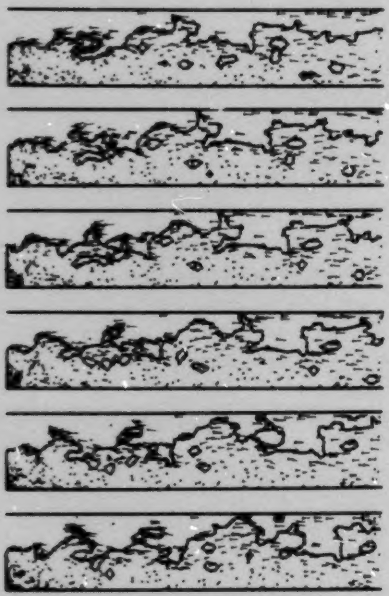


FIGURE 2.6 A sequential series of computer plots displaying velocity fields and flame fronts in turbulent combustion behind a step at inlet Reynolds number of 10000. The combustion is stabilized by a recirculation region behind the step. The unburned gas is a mixture of propane and air at an equivalence ratio of 1/2. [From A. F. Ghoniem, A. J. Chorin, and A. K. Oppenheim, Numerical modelling of turbulent flow in a combustion tunnel, *Phil. Trans. R. Soc. London. Ser. A* **304**, 303-325 (1982).]

steady, planar flame) as one or more parameters exceed critical values for instability of the basic solution. Their significance lies partly in the fact that they represent intermediate modes of propagation of the flame in its evolution from a laminar to turbulent form of propagation. Experimental observations of these transitional modes in their pure form have recently been reported, and the theory thus identifies critical parameter thresholds that separate one form of flame propagation from another. A number of bifurcation analyses using nonlinear perturbation methods have been successful in characterizing these nonsteady and/or nonplanar flames for parameter values near the instability threshold. However, numerical approaches may be used to great advantage in describing these transitional solutions when parameters far exceed their critical values for instability of the basic solution.

2.3 PLASMA PHYSICS

Controlled nuclear fusion provides a possible long-range energy source. As currently conceived, a fusion device must contain a deuterium and tritium plasma for a sufficiently long time for net energy production. The confinement may be effected either by magnetic fields or by simple inertia effects. Inertial confinement of a pellet, coupled with laser or particle beam heating, is a distinct possibility, although the bulk of the world fusion program centers on magnetic confinement of a plasma. The underlying problems in magnetic confinement are the determination of the equilibrium, stability, transport, and heating properties of plasmas under realistic conditions. Numerical modeling and computation represent major tools in this study. In recognition of their importance, the Magnetic Fusion Energy Computing Center has been established at Lawrence Livermore National Laboratory in Livermore, California. This Center is the third largest scientific computing center in the United States, and its sole function is to provide computing capability to the scientists and engineers in the U.S. fusion community. Fusion plasma physics spans a diverse collection of fields, with significant efforts occurring in the fields of Hamiltonian particle dynamics, statistical mechanics, kinetic theories, and dissipative and nondissipative single and multifluid models. The complexity of the problems involved makes computation an integral part of the research and development program for fusion.

Controlled-fusion confinement experiments have indicated that, even in grossly stable configurations, fluctuations may play an important role in determining energy and particle transport. Thus, an understanding of the nonlinear behavior of various plasma models is fundamental to describing such behavior. For both ideal magnetohydrodynamics, a fluid model, and the Vlasov-Maxwell system, a kinetic model, linearized equations have been studied extensively. These analyses are appropriate for describing small-amplitude deviations from a quiescent equilibrium but omit the effects of mode-mode coupling and the onset, properties, and evolution of turbulence. The development of a self-consistent model of plasma equilibrium with fluctuations, stochastic particle and magnetic-field-line behavior, and resulting transport will continue to be an important research area.

Plasma fusion applications present many problems in which the equations of Hamiltonian dynamics appear. These systems describe single-particle phase-space trajectories in the Vlasov-Maxwell theory of collisionless plasmas. In addition, the trajectory of a magnetic field line in a toroidal system is described by a nonlinear Hamiltonian. Thus, the question of the existence and construction of adiabatic invariants, explicitly time-dependent or not, is of fundamental importance for these systems. Significant progress in this area might be made by combining ideas from modern topological dynamics, numerical simulation, and perturbation analysis. For example, if magnetic field lines are ergodic throughout a volume rather than lying on closed invariant surfaces, as is given by the Kolmorogoff-Arnold-Moser theory, then, owing to electron streaming, the thermal conductivity within this volume will be very fast. Thus, such questions as when ergodicity arises and what the properties of Hamiltonian dynamics are under ergodic circumstances impact strongly on these applications.

Since computational modeling of the full three-dimensional plasma equations is out of the question, current work utilizes a range of different compromises, simplifying to different degrees either the physics or the geometry to obtain a number of computationally tractable problems, each of which illuminates in a distinct fashion, a different aspect of the full plasma problem. In spite of these difficulties, the computational approach is a major route to progress on the problem of controlled fusion. The reason is simple. Experiments are expensive and must be supplemented to the maximum extent possible by theory. The theory is highly complex and nonlinear and is obtained by a combination of numerical experiments and physical intuition. Clearly improved computational methods are one of the methods through which progress is achieved in this area. Development of more powerful computers will also be required, as it is hard to believe that smart algorithms will by themselves suffice.

2.4 PARTICLE PHYSICS

The problem is to find the equations that describe the elementary particles of subnuclear physics. This problem is among the most difficult to have been considered seriously by science in this century. In recent years there have been significant gains in our understanding of the mathematical structure of the equations of quantum field theory. An analysis of the mathematical existence question for the quantum ϕ^4 equation

$$\frac{\partial^2\phi}{\partial t^2} - \Delta\phi + m^2\phi + \lambda\phi^3 = 0$$

shows that in space-time dimension $d \leq 3$, the theory exists, whereas in $d \geq 5$, there is no such theory (as would be given by standard methods) except for the trivial case $\lambda = 0$. The method of proof suggests nonexistence for the physical case $d = 4$ as well and offers confirmation from the side of exact mathematical analysis of ideas advanced by theoretical physics. This mathematical confirmation is much more compelling than any confirmation yet offered from experimental physics.

The ϕ^4 model is "near" to the Sine-Gordon equation, which is completely integrable. Among recent results are the discoveries of a large class of stable, localized (in space), periodic (in time) solutions (analogs of the Sine-Gordon breather) and of the existence of breather formation resonances in soliton/antisoliton scattering. There are many related challenging problems in nonlinear mathematics and dynamical systems theory.

The problem with the ϕ^4 equation in $d = 4$ dimensions is one of several reasons for considering in its place quantum gauge fields. A standard approach to the quantization problem reduces it to the existence question for a singular non-Gaussian functional integral over an infinite-dimensional space. In the case of gauge fields the gauge potentials form an infinite-dimensional affine space $\mathcal{A}$ on which the group $\mathcal{G}$ of gauge equivalence acts. The functional integral is only defined over the infinite-dimensional manifold

$$\mathcal{M} = \mathcal{A}/\mathcal{G}$$

This manifold is not flat. The integration over $\mathcal{M}$ has been shown by exact mathematical analysis to require introduction of coordinate patches. Only locally, within a single coordinate patch can $\mathcal{M} = \mathcal{A}/\mathcal{G}$ be regarded as an open subset of Euclidean (Hilbert) space.

One of the methods proposed for understanding integration over $\mathcal{M}$ is to understand the critical points $\Lambda \in \mathcal{M}$. This question leads to a study of *classical* solutions of the Yang-Mills equation and a reduced form of this equation, called the self-dual Yang-Mills equation. Here we are looking at a specific nonlinear elliptic equation in $d = 4$ dimensions. A remarkable analysis has led to a complete classification of its solutions, using methods of geometry, topology, and algebra (fiber bundles, the index theorem, and algebraic varieties).

The development of numerical methods for the study of quantum fields is in its infancy, mainly because the problem is to a large extent out of range of present-day computing machines. Among the methods used on this problem, we mention Monte Carlo integration over a space-time discretized version of $\mathcal{M} = \mathcal{A}/\mathcal{G}$. The discretized problem is called a lattice gauge field, and even after discretization, the dimension of $\mathcal{M}$ is too high to allow evaluation of integrals by direct quadrature. A second approach is to generate series coefficients from cluster expansions of statistical physics and to reconstruct the desired function space integral from a Padé analysis of the coefficients. Other attempts have been based on finite elements and on the renormalization group. It may be that a collaboration of numerical analysts with mathematical or theoretical physicists on this problem would be beneficial.

2.5 CONDENSED-MATTER PHYSICS

2.5.1 Statistical Physics

In this subject, the equation of state, transport coefficients (pressure, viscosity, and thermal conductivity, for example), and other macroscopic properties of matter are related to and derived from intermolecular forces. The area has diverse and important applications, ranging from metallurgy to polymer chemistry to semiconductors and is an active area of research from the points of view of theory, numerical methods, and experiment. Here we limit ourselves to the two mathematical aspects of this subject: mathematical theory and numerical methods.

The equations of statistical physics involve a large or infinite number of degrees of freedom, and so the mathematical theory of use here is analysis over infinite-dimensional spaces. Almost the same mathematical structure arises as in the study of quantum fields, the relationship between the two being that a quantum field is a continuum limit of a statistical physics (crystal or lattice) model.

In a small class of models, including the two-dimensional Ising model, exact solutions are known. A larger but still restricted class of models has been analyzed mathematically with respect to qualitative behavior. One

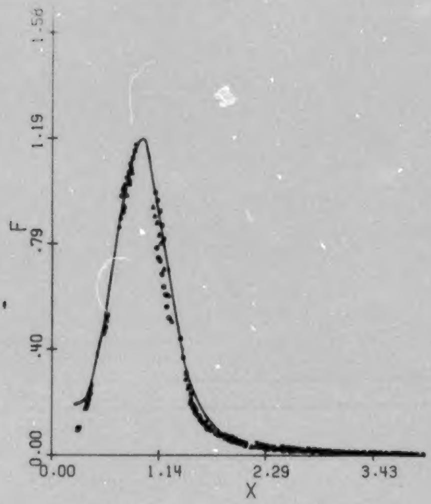


FIGURE 2.7 Monte Carlo simulation of a kinetic Ising model compared with x-ray and neutron defraction measurements on an alloy of 60 percent gold and 40 percent platinum that has been heated and then quenched to 60 percent of its critical temperature. The abcissa is a reduced momentum transfer, and the ordinate is a reduced scattering intensity. (From M. H. Kalos, New York University.)

issue recently addressed in this work was the stability of surfaces, as is relevant to the problem of crystal growth. Another is the effect of aperiodic or random crystal structure on bulk material properties. A striking recent development was the mathematical demonstration of the dipole binding (Kosterlitz-Thouless) phase transition.

The numerical methods for statistical physics are basically of three types. In molecular-dynamics calculations, one takes a large number of particles and follows their motion by integration of the ordinary differential equation

$$m\frac{d^2x_i}{dt^2} = F_i(x_j - x_i), \quad i = 1, \ldots, N$$

defined by the intermolecular forces F_i. This method is "exact" in its treatment of intermolecular forces, to the extent that they are known and that quantum effects can be neglected, but it is approximate in its treatment of statistics, since there are computer-dictated limits on the number N of particles that can be included.

Next we mention the method of series expansions, applied to the calculation of the equilibrium distribution $d\omega$ and the partition Z, which typically has the form

$$d\omega = e^{-V(x)} \prod_i dx$$

and

$$Z = \int d\omega$$

where V is the intermolecular potential energy. Then thermodynamic functions such as pressure emerge as derivatives or logarithmic derivatives of Z with respect to the parameters (e.g., in V). If the potential energy

$$V(x) = \sum_{i<j} U(x_i - x_j)$$

is a sum of pair potentials U then the identity

$$e^{-U} = 1 + (e^{-U} - 1)$$

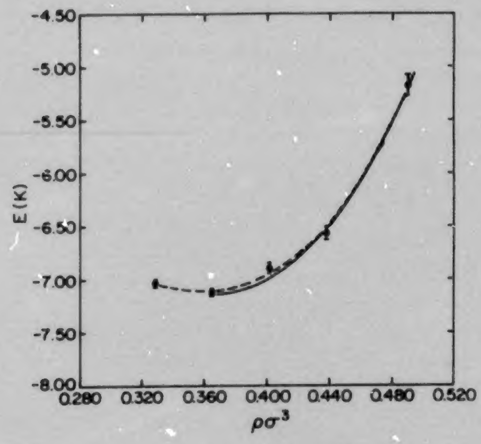


FIGURE 2.8 Energy of liquid helium as a function of density. The broken line and points with errors show results of the Monte Carlo quadrature of the many-body nonrelativistic Schrödinger equation. The solid line is a fit to the experimental data. (From M. H. Kalos, New York University.)

substituted in the definition of $d\omega$ above yields an expansion that is rapidly convergent, where

$$|e^{-U} - 1| \ll 1$$

i.e., where $U \simeq 0$. This is the region of noninteraction, and so series expansions are especially useful to give weak corrections, for example, real gas corrections to an ideal gas. The expansions appear to converge up to critical points and with considerable work have been used to extract information on the equation of state in that region.

Monte Carlo methods are used in the quadrature of very large-dimensional spaces, such as the determination of $d\omega$ above, as well as in the direct simulation of stochastic systems. These methods have become an experimental tool of mathematical physics. In studying the qualitative and quantitative behavior of a highly idealized model such as the Ising model in equilibrium or very far from equilibrium, or of lattice gauge theories, continuum and lattice models of polymers, and atomic models of quantum liquids and solids, one can carry out numerical studies in which the high-dimensional (i.e., many-body) character of the problem is not distorted.

In application to the calculation of the equilibrium distribution $d\omega$, the essence of the Monte Carlo method is as follows: Starting from an arbitrary point in a given ensemble, one modifies a single particle position x_i "at random" but usually so as to lower the potential energy V, occasionally so as to raise V. After enough such elementary steps, convergence to the distribution $d\omega$ is obtained. As described here, the method is extremely simple, and complications arise from the necessity to obtain convergence in a reasonable time for realistic problems.

Perhaps the most significant success has been in the microscopic theory of classical fluids, where Monte Carlo modeling has provided the "experimental" basis for the accurate expansion in $|e^{-U} - 1|$ mentioned above. Another conspicuous success is the extraction of critical exponents by joining ideas of the renormalization group to Monte Carlo simulation. Figure 2.7 shows Monte Carlo simulation of a kinetic Ising model compared with scattering measurements on a real alloy.

Figure 2.8 shows how Monte Carlo methods applied to the many-body nonrelativistic Schrödinger equation give a quantitative account of the energy of (real) liquid helium as a function of density.

2.6 GEOPHYSICAL APPLICATIONS

Out of a wide range of geophysical applications we limit ourselves here to three modeling problems in connection with the discovery and production of petroleum. Mathematically the discovery process is an inverse problem (see Section 3.6)—that of constructing geologic maps using seismic signals, which in turn are generated by vibrations or explosions at the surface of the Earth. As the signals penetrate the Earth, they cross layers of differing density. This causes reflected signals to be returned to the surface, where they are then recorded and analyzed. The raw data are very noisy, owing to irrelevant near-surface density fluctuations. The noise is removed by averaging signals from neighboring receptors or from neighboring source locations. Then multiple reflections must be subtracted, and a compensation (called normal moveout) must be introduced for effects of nonvertical signal propagation. Reflection from nonhorizontal layers generates complicating shear waves as well as pressure waves. The subtraction of multiple reflection signals can be based on Fourier analysis in a half-space and a Wiener-Hopf factorization.

The correction for nonvertical signals can be based on a reduced Helmholtz equation, $(-\Delta + k^2 + v)u = 0$, but in order to focus on signals moving in only one direction (either up or down), one takes first a square root and then a power series expansion of the square root. This process is known as the parabolic approximation and leads to the familiar Schrödinger equation. Alternatively, the analysis can be based on ray tracing and the solution of ordinary differential equations. The numerical problem is to implement these steps efficiently, in view of the large amount of data to be analyzed.

The production problem is to describe the flow of oil, water, chemicals, and/or heat in a porous sandstone layer. The equations to be solved are a coupled system of nonlinear parabolic equations. Generally the equations describe mass conservation of individual species, and typically some are nearly elliptic whereas others are nearly hyperbolic. In the hyperbolic equations, coherent shock and rarefaction waves describing oil banks, absorption fronts, and flame fronts may form (see Sections 3.2 and 3.3). Depending on a dimensionless number known as the mobility ratio, heterogeneities, and geometrical effects (convergence versus divergence), the fronts may become unstable with respect to the formation of fingers (see Section 2.1).

Critical issues in this problem are the efficient solution of large sparse linear systems arising from space and time discretizations and the control of numerical instabilities in the solution methods. The physical in-

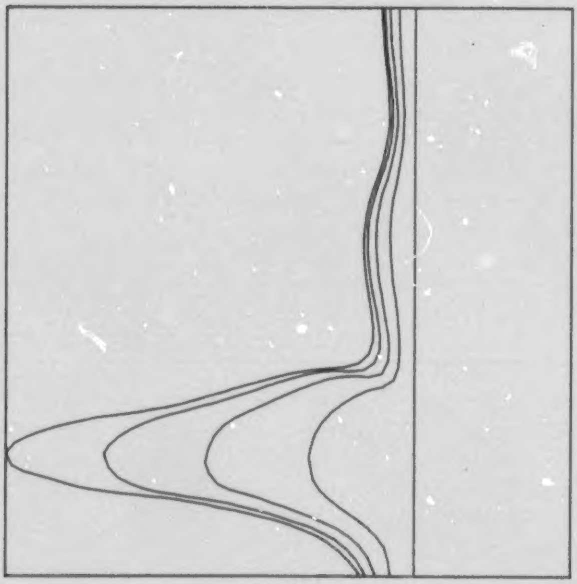


FIGURE 2.9 Successive time steps in the movement of an oil-water interface toward a producing well. The view is a vertical cross section, with the well located on the left boundary of the computational region. The instability is caused by three factors: by a heterogeneous conducting channel near the bottom of the reservoir, by the converging cylindrical flow pattern near the producing well, and by the better flow properties of the less viscous displacing fluid (water). [From J. Glimm, B. Lindquist, O. McBryan, and S. Yaniv, Statistical fluid dynamics II: the influence of geometry on surface instabilities, in *Frontiers in Applied Mathematics*, Vol. 1, R. Ewing, ed., SIAM, Philadelphia, Pa. (to be published).]

stabilities mentioned above are controlled by the use of heat (to make the oil flow more easily) or the use of a heavier pushing fluid (polymer-thickened water in place of water or water and CO_2 in place of CO_2).

The third modeling problem we discuss is the process of lifting the oil to the surface of the Earth. Because of the sudden drop in pressure, considerable gas will typically come out of solution, and the resulting two-phase mixture is in the droplet or mist regime mentioned in Section 2.1. In contrast to the case of reservoir flow, even the basic equations for two-phase flow in a pipe are not well understood.

2.7 METEOROLOGY

Accurate forecasting of the movement of large-scale weather patterns is clearly an important problem. Here we mean the tracking of highs and lows on the order of 1000 kilometers in diameter. In addition, we are also concerned with the prediction of cloud patterns, precipitations, temperature, and other elements of the weather in as much detail as possible. Global predictions of the atmospheric flow are now made routinely at as many as 12 levels in the troposphere and stratosphere.

By studying dynamic models of the atmosphere, estimates have been made of the sensitivity of the atmosphere to small perturbations, often quantified in terms of the error doubling time. If two initial states of the atmosphere differ by random variations of 1°, then it is found that the resultant states will differ by 2° in about 3 days and by about 4° in about 6 days. Hence, meteorologists have said that the weather is unpredictable for periods of more than 2 to 3 weeks. But, the forecasters are still far from being able to predict the weather accurately for even 1 week. The best results are currently obtained by the European Centre for Medium Range Weather Forecasting, whose 4-5 day forecasts are currently superior to those of the U.S. National Weather Service.

The accuracy of short-range predictions is limited by four somewhat distinct factors:

1. Initializations: (a) The accuracy and completeness of observational data and (b) the compatibility of these data with the mathematical model, which is, of course, a simplified representation of the atmosphere.
2. The limited number of grid points or spectral components used in the truncated, i.e., numerical, model as a result of limited computer power.
3. Missing or severely truncated physical processes such as cloud dynamics, proper representation of turbulence, and radiation fields, leading to inadequacy of the mathematical model describing the atmosphere.
4. The inherent finite limits of predictability of certain types of nonlinear dynamical systems such as the atmosphere. (Compare the previous paragraph.)

The study of problems related to the reduction of the influence of these factors is at the heart of most research that is directly related to the improvement of weather prediction.

The sparsity and inaccuracy of observational data [1(a)] are being partially overcome by the use of weather-observing satellites. Concerning 1(b), considerable research is currently directed toward the analysis and filtering of the observed data so as to make them compatible with numerical models. Items 2 and 3 are closely related since, in a general way, the lack of a complete representation of all physical processes is related to the incomplete numerical resolution of the mathematical model. Such physical processes include cloud dynamics (and the associated cloud physics), boundary-layer dynamics (including detailed features of the terrain and local heat, moisture, and dust sources), and detailed radioactive processes. In item 4 a new concept, "finite limits to predictability" has emerged from the work of E. N. Lorenz, namely the idea that the atmosphere and perhaps certain other dynamical systems may have finite limits of predictability regardless of the accuracy and detail of their initial conditions and the accuracy with which they are computed. Lorenz concluded from a simplified model that hydrodynamical systems with an energy spectrum (in the customary sense) having a power-law exponent greater than -3 (e.g., $-5/3$) should be unpredictable in detail after a finite time. He suggests a time of about 15 days for the atmosphere, whose large-scale energy spectrum seems to have an exponent of about -2.8, with smaller scales (i.e., less than say, 20 km) having the $-5/3$ power law associated with homogeneous turbulence. This question of predictability is clearly related to that of the stability of hydrodynamical systems and to modern theories of bifurcation and chaos (see Section 3.5).

A large component of atmospheric research is concerned with topics that have little direct application to forecasting. Their motivation may lie in basic scientific inquiry or in applications to other disciplines, e.g., radio-wave transmission for satellite communications. They may involve the study of fundamental hydrodynamic phenomena or other physical processes several steps removed from specific application. In all of these studies we find extensive use of analytical and numerical modeling of physical systems and processes. In addition, a wide variety of statistical approaches are used in all areas of atmospheric research.

Let us mention a few more areas of study. In addition to the prediction of large-scale weather patterns, computers are being used in limited regions to study the development and movement of smaller-scale disturbances, such as hurricanes, thunderstorms, and tornadoes. Here adaptive grid methods are used (see Section 4.2). It is hoped, for example, that a better understanding of the details of these destructive phenomena will lead to the possibility of altering their course and development.

On the longer time scale, where seasonal forecasts of average rainfall and temperature are made over large regions of the globe, there are at present several potentially useful, but unproven ideas. Here, however, some new mathematical and physical insight is needed in order to develop a satisfactory "average" system of equations. This is an important open problem.

On the still longer time scale of decades and beyond, determining the effect of our mechanized civilization on the environment is a basic problem. Significant progress has already been made, through the use of simple climate models in conjunction with paleontology, astronomy, geology, and volcanology, in efforts to understand the factors that influence irregular alternations of ice ages and interglacial periods. These statistical-dynamical climate models will be essential for predicting the long-term effects of the observed increase in carbon dioxide and similar problems that will almost certainly arise as our industrial civilization expands.

2.8 ASTROPHYSICAL APPLICATIONS

Astrophysical studies pose a wide range of problems for mathematical and computational analysis. The underlying physical theories include hydrodynamics, magnetohydrodynamics and plasma theory, radiative transport theory, atomic and nuclear physics, and general relativity theory, and hence various comments made in other applications sections of this report apply to this area.

In recent years considerable progress has been made in theoretical and numerical studies of a number of astrophysical topics, as, for instance, the study of stellar interiors, the formation of stars and galaxies, the spiral structure of galaxies, the physics of supernovae and the evolution of supernovae remnants, the formation of the solar system, and the behavior of binary star systems, to mention just a few. The computational approaches may range from relatively simple simulations to the numerical solution of complex systems of partial differential equations.

As an example of the first type, simulations have been applied to the study of star formation in a galaxy. It may be assumed that when a massive star becomes a supernova the shock wave emanating from it can compress the surrounding interstellar gas creating new stars. If at least one new star is also a massive star the phenomenon can repeat, leading to a chain reaction in the creation of stars. This is equivalent to a direct percolation problem, and, as is typical for such problems, phase transitions are involved. This is a nonlinear problem with a complicated structure in space and time. Accordingly, analytic techniques are difficult, whereas computational simulations are relatively straightforward and lead to the development of realistic model galaxies.

As a second type of example we mention a problem that is amenable to considerable mathematical analysis as well as to computational attack. This is the question of the spiral structure of galaxies. The so-called density wave theory approaches this question as a dynamical problem in the form of the gravitational instability of a galactic dish with respect to spiral modes. There are three basic approaches in the calculation of spiral structures of galaxies on the basis of density wave theory that may be characterized loosely as the stellar model, particle model, and fluid model.

The stellar model represents the classical approach in the study of stellar systems. In brief, a galaxy has a stellar component and a gaseous component. The latter usually has a sufficiently small mass to be negligible in first approximation. The basic equations governing the behavior of the stellar component are the Boltzmann equation, usually in collisionless form when close encounters between stars are omitted, and the Poisson equation for the gravitational potential. In a sense, these equations are much simpler than the Vlasov equations of plasma physics, but their numerical solution nevertheless poses challenging questions.

In the particle model, the stellar component is considered as a very large but finite number of particles. As in our first example, the computational approach then assumes the form of a simulation process. In brief, the motions of the individual stars are followed, and their gravitational field is calculated by a self-consistent evaluation of the field. This technique has provided valuable qualitative information. But the number of stars in these models is usually of the order of $10^{11\pm1}$, and hence, by necessity, numerical simulations are extremely limited in accuracy and provide only few quantitative data for specified galaxy models.

In the third approach, the stellar system is considered to be a continuous medium. In this setting one may then study the characteristics of wave patterns over the galactic disk and then dependence on the mass distribution. In particular, the spiral structure of galaxies may be explained in terms of spiral wave patterns of some kind. Such stationary wave patterns over a field of differential rotation are to be expected; in fact, hydrodynamic waves over shear flows are known to exist for some time especially in the form of self-excited modes. The general form of the resulting theory of spiral galactic structures requires elaborate computational techniques. At the same time, asymptotic approaches have provided analytic results that have led to a better understanding of the dynamical mechanisms despite their limitations in accuracy and in the types of galaxies covered.

As noted earlier, these are only some examples of the many different types of problems in astrophysics that relate closely with applied and computational mathematics. Many of these problems involve extremely wide ranges in length and time scales. For example, calculations of stellar evolutions have to range over billions of years, while the dynamics, say, of the supernovae phase takes place within milliseconds. Similarly, the size of a neutron star differs by substantial orders of magnitude from the size of its corresponding relevant gravity field. Thus, in particular, the mathematical and computational difficulties, discussed in Section 3.2, are especially applicable here. Moreover, the wide range of the underlying physical theories leads to many substantially different types of mathematical models, which in turn require very different computational techniques.

2.9 STRUCTURAL MECHANICS

During the past two decades, the use of computers has transformed large parts of solid mechanics into practical tools for a multitude of technological developments. Sophisticated computational software is employed throughout the nation's industries and research laboratories in the analysis and design of structures and mechanical equipment. There is a strong interaction between applied mathematics and solid mechanics. Mathematical analysis has provided insight into model formulation and the development of powerful numerical methods; and, vice versa, novel engineering approaches have led to new research areas in applied mathematics.

In the case of linear problems there exists now a relatively broad experience in computing solutions for a range of problems concerning the behavior of solid bodies subjected to specified loads. In general, the computed results are considered reasonably reliable, and they have been corroborated over a period of time by observation and practical experimentation. There appears, however, to be a growing need for the development of computable error estimates that can provide a realistic check on the solution accuracy. Such *a posteriori* bounds have been shown to be feasible; but their applications to large, realistic problems in solid mechanics still requires considerable research and software development. The general availability of economical *a posteriori* estimates would make possible the consistent use of adaptive mesh-refinement techniques that would reduce the cost of data preparation by the users and make it possible to generate near-optimal solutions for a given amount of computational expense.

The general trend in computational solid mechanics today is toward extending the computational methodology to nonlinear problems. Sources of nonlinearity in structural problems are (1) geometric nonlinearity due to nonlinear strain-displacement relations, (2) material nonlinearity due to nonlinear constitutive equations, (3) force nonlinearity due to nonlinear stress boundary conditions, and (4) kinematic constraint nonlinearity due to nonlinear displacement boundary conditions. The source of nonlinearity affects the form of the resulting nonlinear equations and, hence, influences the effectiveness of the solution techniques.

The numerical analysis of all of these nonlinear problems is not yet at a satisfactory stage. Many computer programs for such problems exist, but the mathematical basis for most of the methods used is insufficiently understood, and there is little known about the accuracy of the computed results. Moreover, in the case of nonlinear problems, few numerical computations can be supplemented with sufficient experimental experience.

The situation is still best understood in the case of finite elasticity. Even there the mathematical theory of the underlying equations is incomplete, and the approximation theory for these equations is generally based on various simplifying assumptions that may or may not be valid for a particular problem.

The state of the art in elasto-dynamic problems is in even worse shape. It is known that multiple solutions may exist and shock waves can develop. Moreover, not all solutions are necessarily physically relevant. The questions of how to model such phenomena numerically and how to determine the physically realistic solutions are as yet largely open. When it comes to problems in finite plasticity even less is known. Although there has been much progress in this area during recent years, no satisfactory and complete mathematical model is available as yet. Especially, there are profound mathematical and computational difficulties in modeling phase changes, viscous effects, cracks and singularities, the growth of cracks under dynamic loading, and the identification and implementation of physically reasonable constitutive equations describing these materials.

2.10 NONDESTRUCTIVE TESTING AND TOMOGRAPHIC RECONSTRUCTION

There is a pervasive need in technology to evaluate quantitatively the integrity and the remaining reliable lifetime of components and structures, e.g., from bridge girders to high-performance ceramic turbine disks. In the past decade considerable progress has been made. This developing technology is called nondestructive evaluation (NDE) to distinguish it from older nonquantitative nondestructive testing practices. NDE presents challenges to the applied mathematical sciences on many levels. A few of the more important and topical problem areas are mentioned here.

In NDE applications a component is often subjected to some sort of penetrating radiation with the aim of deducing information about its internal state from a measurement of the radiation field external to the part. Examples include the use of ultrasonic radiation, x rays, and neutrons. Because of its flexibility, relative cost, and safety, ultrasonic methods are often used in NDE applications. The deduction of information about flaws from the incident and scattered ultrasonic fields relies on the solution or approximate solution of the inverse scattering problem for elastic waves. In some regimes it is possible to develop and adapt imaging techniques to the ultrasonic setting. In either case information about defects must be obtained from band-limited noisy data. A fundamental limitation to our current ability to utilize ultrasonic techniques broadly is our limited understanding of the elastic inverse scattering problem in either the frequency or the time domain.

In other important NDE applications, electrical currents are induced in a material. These currents produce fields that vary depending on whether a defect, e.g., a crack, is present in the material. The utilization of these so-called eddy-current techniques depends on the ability to infer information about the defects from the measured fields they produce. This again is an inverse problem that is imperfectly understood.

Passive methods in NDS are also widely used. For example, when a pressure vessel or aircraft is in service, a crack once formed may grow and propagate. This will be accompanied by the release of acoustic energy. This energy can in turn be monitored at selected sites. The problem then becomes one of identifying and classifying the sources of these sound patterns using acoustic emission studies, an increasingly important technique in NDE. In mathematical terms the problem is the so-called inverse source problem, which is beset with the same type of difficulties that the inverse scattering problems possesses. Sparse, noisy data often taken at highly nonoptimal locations are the raw information from which source characteristics must be deduced.

The techniques of NDE have application in other areas, and much can be learned in other applications fields that is valuable to NDE. For example, there is a close connection between the need for inverse scattering results in geophysics and NDE and acoustic imaging results in NDE and biomedical applications. An area of great success in medical applications, tomography, can provide useful information in selected NDE applications.

The greatest success of tomography has been in medical applications such as the CAT (computer assisted tomography) scanner. Unlike ordinary x-ray technique, which masks important features by superposing on a single picture information on planes perpendicular to the beam, computerized x-ray tomography provides pictures of individual thin slices through the body. Several hundred parallel x-ray pencil beams are projected in the plane of the slice, and the attenuation of the x rays in each beam is measured separately and recorded. The procedure is repeated for many different beam directions. An elaborate calculation then permits approximate reconstruction of the x-ray attenuation density as a function of position within the slice.

The idealized mathematical problem is the reconstruction of a function of two variables from its integrals along lines. This problem, as well as its three-dimensional version, was solved by Radon in 1917 and later rediscovered in various settings such as probability theory (recovering a probability distribution from its marginal distributions) and astronomy (determining the velocity distribution of stars from the distribution of radial velocities in various directions). Of course, much work was needed to adapt the Radon inversion formula to the incomplete information available in practice. Various algorithms for the numerical inversion of this ill-posed problem have been proposed, with the present trend favoring the so-called convolution algorithm on account of its speed and accuracy. Each area of application has, however, its own requirements and may need a modification of existing reconstruction algorithms or even a custom-made one. Some algebraic methods, for instance, can easily incorporate *a priori* information about the object to be reconstructed.

Recent advances in medical tomography include nuclear magnetic resonance (NMR) tomography and positron emission tomography (PET). In NMR strong magnetic fields are used to affect the nuclear magnetic spin rate of hydrogen atoms. By varying the fields and their direction, the plane integrals of the density of hydrogen can be measured and the density reconstructed by an algorithm based on the above three-dimensional version of Radon's theorem. The technique is now regarded as competitive with x-ray tomography for many purposes; and, of course, it is not ionizing. The advantage of PET over CAT is that metabolic processes can be followed. A compound such as glucose is made using carbon-11 atoms, which emit positrons. Photons resulting from the annihilation of an emitted positron with an electron are detected by a bank of detectors that can record coincidences. Recently, algorithms based on probabilistic arguments have been proposed for the PET reconstruction problem.

2.11 MATHEMATICAL MODELS IN THE BIOLOGICAL SCIENCES

The biological manifestations of the physical laws of the universe present us with a rich variety of new phenomena that require the devlopment of new mathematical tools and computational methods. We shall discuss just a few examples of mathematical research in cardiovascular physiology and neurophysiology, with the knowledge that there are many other areas of biological sciences in which mathematics and computing are fruitfully applied.

Blood flow in the heart obeys the incompressible Navier-Stokes equations, which, in turn, are simply a statement of Newton's laws in differential form (see Section 2.1). The distinctive biological character of the problem comes, however, from the moving boundaries that are in contact with the blood. These include the muscular heart walls and the

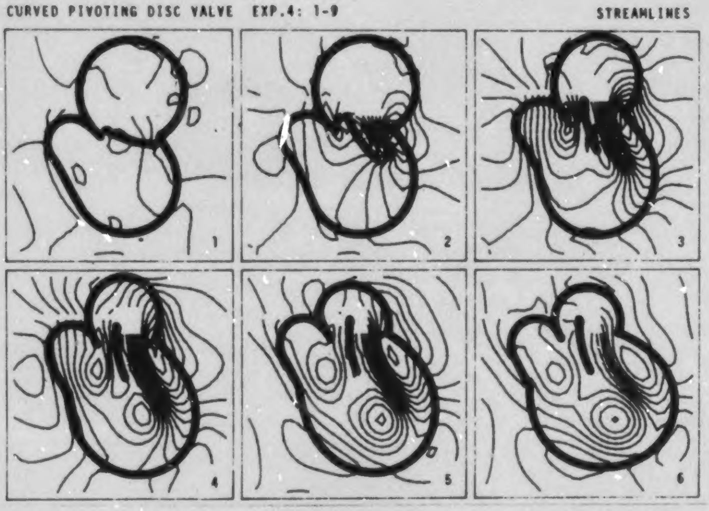


FIGURE 2.10 Computer-generated plots showing the predicted opening movement of a curved pivoting-disk valve mounted in the mitral (inflow) position of the left ventricle. The curvature makes the valve open more widely than a straight valve pivoted at the same point. It also helps to prevent stagnation in the smaller opening of the valve. [From D. M. McQueen and C. S. Peskin, Computer-assisted design of pivoting-disc prosthetic mitral valves, *J. Thorac. Cardiovasc. Surg.* (in press).]

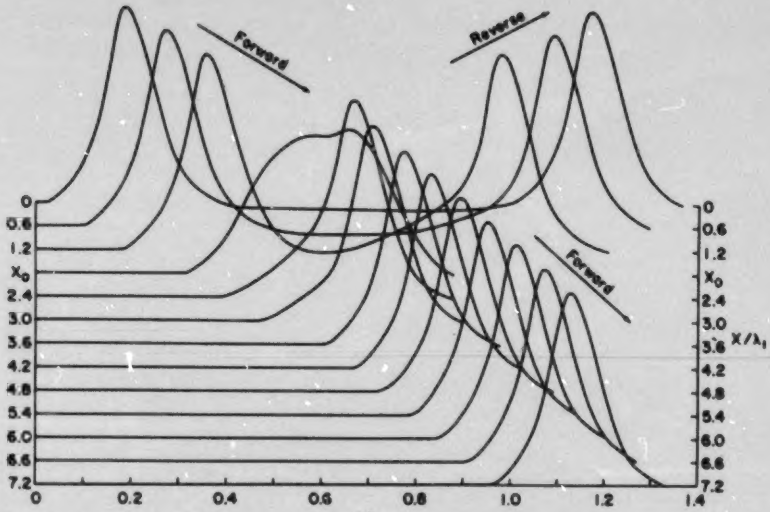


FIGURE 2.11 Transmission and "reflection" of a nerve impulse at a junction where the diameter of the neuron suddenly increases. The plots show computed voltage as a function of time at equally spaced positions. The junction is at $x = x_0$, and the ratio of diameters there is 2.5:1. Note the increase in propagation speed for $x > x_0$. A reflected wave is set up when the larger fiber re-excites the smaller fiber after the refractory period of the smaller fiber has elapsed. [From S. S. Goldstein and W. Rall, Changes of action potential shape and velocity for changing core conductor geometry, *Biophysical J.* **14**, 731 (1974).]

elastic heart valve leaflets. The motions of these boundaries are not known in advance; they must be computed along with the motion of the fluid.

These considerations have led to the development of a computational model of the left heart that can be used in the computer-aided design of artificial heart valves. In this model, the fluid equations are solved by finite-difference methods on a regular, square mesh (see Section 3.4). The boundaries are represented in Langrangian form as a collection of moving points. Coupling coefficients between boundary markers and fluid mesh points are computed with the aid of an approximation of Dirac's δ-function. This computer model (Fig. 2.10) has been used in the design of prosthetic heart valves to remedy problems of stagnation and blood clotting in the smaller opening of the valve. The model has also been helpful in the study of disease processes, providing, for example, a possible explanation for mitral valve prolapse.

Just as the flow of blood in the heart is ultimately governed by Newton's laws, the conduction of electrical signals along nerves is ultimately governed by Maxwell's equations (Figs. 2.11 and 2.12). Here also, nature provides a peculiar boundary condition that leads to entirely new phenomena. In this case the boundary condition comes from certain voltage-dependent channels located in the nerve membrane. These introduce a nonlinearity, and the equations of nerve conduction take the form of nonlinear diffusion equations—the Hodgkin-Huxley equations. Without

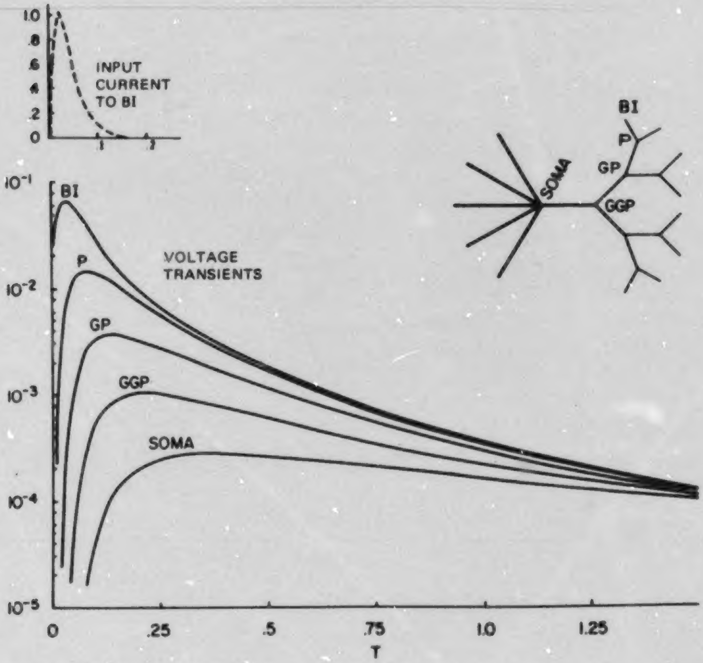


FIGURE 2.12 Computed electrical signals at the input end of a neuron. A brief pulse of current is applied at the periphery of a tree, and the resulting voltages are computed (logarithmic scale) at the input (BI), at successive branch points (P, GP, GGP), and finally at the cell body (SOMA). [Modified from J. Rinzel and W. Rall, Transient response in a dendritic neuron model for current injected at one branch, *Biophysical J.* 14, 759 (1974).]

the nonlinearity, signals introduced at one end of the nerve would decay rapidly; because of the nonlinearity such signals evolve into a specific waveform that propagates at a constant speed without distortion. This waveform is called the nerve impulse, and it is the basic unit of long-distance communication in the nervous system.

Currently, there is a wide range of mathematical, computational, and physiological research activity related to the Hodgkin-Huxley equations. Mathematically, there is extensive research on the basic theory of nonlinear diffusion equations. A particularly fruitful approach here has been the use of piecewise linear models that expose the basic structure of the equations. Singular perturbation methods have also been useful because the equations exhibit a disparity of time scales.

An important physiological enterprise is the modification and application of the Hodgkin-Huxley equations to other excitable tissues. In the heart, for example, equations of the Hodgkin-Huxley type describe the electrical processes that generate the cardiac rhythm and coordinate the heartbeat. Mathematicians are just beginning to use these equations as a basis for a theory of the abnormal rhythms of the heart, of which the most serious is ventricular fibrilation. This theory has connections with recent work on chaotic dynamical systems and transition to turbulence: it appears that fibrilation is directly analogous to turbulence. This work has enormous practical significance, since the principal cause of sudden death following heart attacks is ventricular fibrilation.

Progress has also been made in the modeling of the input to the neuron (whose output signal is the nerve impulse). The neuron integrates information received through a tree of dendrites in which the signaling mechanism is often described by the linear diffusion equation with leakage. Mathematical modeling of the dendritic tree has had a substantial impact on experimental neurophysiology. One reason for this is that dendrites are too small to be penetrated with microelectrodes. Thus the neurophysiologist can only record voltage or inject current at the cell body and is forced to rely on the theory to indicate the significance of these measurements with respect to activity in the dendritic tree.

Some major successes of the theory are as follows:

1. Elucidation of the dramatic differences between effects of a synapse close to the cell body and effects of a similar synapse far out in the dendritic tree.
2. A possible explanation of the role of dendritic spines in learning and memory.
3. Prediction of the existence of dendro-dendritic synapses based

on a mathematical model of field potentials in the olfactory bulb. Such synapses, previously unheard of, were subsequently found in electron micrographs. This work led to a fundamental new concept of local information processing in an "analog" rather than a "digital" mode, i.e., without nerve impulses. Such processing is important in neural networks such as the retina. Indeed, an extensive mathematical theory of the retina has been developed, and this is another exciting area of current research.

2.12 ELECTRONIC COMPONENTS

The design and fabrication of modern integrated circuits is a complex process. The number of devices that one can put on a chip depends on the size of the chip and how small one can make its features. Over the years the largest increase in the number of devices on a chip has resulted from the continuing reduction in feature size and with this a reduction in device size.

Consequently, process and design engineers have had continually to redesign the process steps and then recalculate the resulting device characteristics to ensure good electrical behavior. This has had to be computational because the equations are mathematically intractable and a trial and error approach is prohibitively expensive and time-consuming. Moreover, experimental techniques tell us only what happened, not why. Effective device design depends on determining both the what and the why by varying the problem parameters in the computational model.

The mathematical models on which the theory of semiconductor devices rests are differential equations that describe the flow of current (holes and electrons) under the influence of electric fields. When feature sizes were large, the devices could be treated as though they consisted of plane surfaces and edge effects could be neglected. This allowed the development and successful use of one-dimensional analytical models obtained by solving a system of three coupled, nonlinear ordinary differential equations. As device sizes shrunk, these models became more complicated and less accurate as edge effects became more important. In very large-scale integration where device dimensions have reached a few micrometers, these models are no longer adequate, and the coupled, nonlinear, partial differential equations must now be solved in two and sometimes three dimensions. These differential equations consist of a nonlinear Poisson equation that describes the potential of the electric field and two nonlinear transport equations that describe the motion of the holes and the electrons. Moreover, the smaller sizes have made some physical effects important whereas they were previously neglected. This results in further complications to the basic equations.

Partial differential equations play an increasingly important role in simulating the fabrication processes. The transistors in a chip are formed by implanting certain dopant ions into selected areas of the chip. Subsequent high-temperature processes, such as growing an oxide layer, will cause these atomic impurities to diffuse. Their final distribution is an important factor in determining device characteristics. Insights into these fabrication processes are especially important for increasing the yield of reliable devices, which is a critical factor in their economic viability.

The design of the overall circuit to be placed on a chip leads to large systems of nonlinear differential equations that need to be solved numerically. Then the efficient layout of the circuit on the chip introduces combinational and graph theoretical problems, which again pose formidable computational problems.

3. COMPUTATIONAL AND MATHEMATICAL DIFFICULTIES

Computational mathematics and modeling is a relatively young science, one that is expanding rapidly. The success and importance of the field stems from the fact that its application provides the possibility of tackling significantly more complex and difficult problems than would otherwise be possible. Perhaps the greatest opportunity provided by a computational approach is that it opens the wide realm of strongly nonlinear phenomena to systematic, relatively accurate, and efficient modeling, improving the chance that important phenomena can be isolated and analyzed. Nonlinearities pervade nearly all aspects of applied mathematics, and to a large extent these nonlinearities are responsible for the difficulties that are encountered in computational modeling. Our purpose in this chapter is to explore the source of some of these difficulties. In Chapter 4, we will discuss the direction of some of the computational research needed to resolve the problems.

3.1 DEGREES OF FREEDOM

There are several reasons for the degrees of freedom in a model, and hence the size of computational problems, to increase. One is that we attempt to increase the accuracy and complexity of our representations of the physical conservation laws. Increased degrees of freedom come either from increasing the number of dependent or independent variables. For example, in chemical models the number of dependent variables is increased by increasing the number of chemical species considered. An obvious need for increased independent variables comes from the need to represent phenomena in two and three spatial dimensions. However, even higher-dimensional problems arise when the independent variables are not the spatial coordinates but are various state descriptors; such higher-dimensional problems are common in physics and chemistry. Unfortunately, the direct application of numerical methods that work well in one or two dimensions often are not usable in three dimensions. Therefore, increasing the degrees of freedom may require significantly different algorithms.

Another way to increase the degrees of freedom in problems is to allow the possibility of multivalued solutions. Certain physical systems allow the solutions to bifurcate, a phenomenon discussed in Section 3.5. Other systems have hysteresis or "history-dependent" properties. In these problems the solutions depend not only on the boundary conditions but also on the path that the transient solution follows. Structural dynamics models for plastic materials in which the stress depends not only on the strain but on the straining rate as well exhibit this behavior.

Consider an example to quantify the magnitude of the computational requirements for multidimensional problems. First suppose we want to follow the evolution of a chemical model having N chemical species. Suppose also that the problem is stiff (see Section 3.2) so for each time step in the evolving system we solve N nonlinear algebraic equations in N unknowns. Even for models with a large number of species this is a relatively straightforward task. However, if we now want to introduce transport phenomena, such as fluid mixing, the problem has to include the spatial dependence of each chemical species.

For a one-dimensional case assume that we use I spatial mesh points and that we estimate what each species will do on the basis of its current local value and that of its immediate neighbors (a three-point spatial stencil involving all species). We now have NI unknowns and a nonlinear system that has $3NI$ nonzero entries in each equation. It is typical to have 40 to 50 species and to require 100 mesh points to resolve the species concentrations accurately. In this case over three quarters of a million words of memory are needed just to store the approximating local linear system along with the solution. This alone is larger than the fast-access memory of most modern computers. Suppose further that the same model is to be posed in two dimensions on a $I \times I$ mesh and in three dimensions on an $I \times I \times I$ mesh. The solutions themselves require NI^2 and NI^3 words of storage, respectively. Worse, the totality of coefficients in the typical linear system will be $5N^2I^2$ and $7N^2I^3$. It is of practical interest to want solutions to three-dimensional combined kinetics and transport problems. However, even for a modest system of 20 species and 50 mesh points per spatial dimension, 2.5 million words are needed to store the solution alone. An additional 350 million are required to store the coefficients of the linear system. (For comparison, we note that the largest computers currently available have 4 million words of fast-access memory.) Moreover, in the high-dimensional cases, the linear system is not conveniently structured for efficient solution.

Clearly a major problem in solving high-dimensional systems of partial differential equations is that after discretization the resulting system of approximating linear equations can be much too large to be solved effectively by direct means. Except in simple cases the resulting equations have to be solved iteratively, and, especially for strongly nonlinear equations, the convergence properties of the iterative process may be a major concern.

Operator splitting methods, such as alternating direction implicit (ADI) (see Section 4.7), also provide a current effective approach for high-dimensional problems. The approach here is to alternate the solution of a set of lower-dimensional problems. The alternated problem approximates the original problem with sufficient accuracy, but the set of lower-dimensional problems is much more easily solved, even in aggregate. Again convergence and accuracy properties must be established in all but the simplest of cases.

For some problems it may be more efficient to depart from the conventional ideas of discretization on a mesh network and consider instead mesh-free methods or (see Sections 4.8 and 4.9) Monte Carlo methods. Unknowns can be changed: instead of the amount of material at a given location, one can ask for the amount of a given wavelength in the solution as a whole. In fluid mechanics, vortex methods could be a more efficient approach. Such methods reduce the size of the linear algebra problems, in comparison with the mesh-oriented methods, if the new unknowns carry all the important information desired.

Decisions about which methods are most effective may depend strongly on advances and changes in computer architecture. Since new architectures, such as vector and parallel processors, are now evolving, the numerical analyst has to re-evaluate his approaches periodically. Also, considerations such as the relative cost of memory versus central processor time can bear heavily on decisions regarding algorithms.

3.2 DIFFERENT TIME AND LENGTH SCALES

In principle a model can contain important length scales that range from the size of an atom to the size of the universe. In practice, however, we limit the range of scales by approximation (see, for example, Section 3.7). Nevertheless, it is often the case that mathematical models of physical processes are characterized by the simultaneous presence in their solution of significantly different time and length scales. The solutions to these models will have regions of strongly localized behavior, such as shocks, steep fronts, or other near discontinuities. Therefore important topics of research in numerical analysis are the consideration of such circumstances and the development of efficient theories and methodologies for their computational solution. Indeed, we often find situations for which solutions are not possible, or at least not practical, without the application of specialized methods to deal with the multiple characteristic scales.

Fluid mechanics and chemical kinetics are two areas that provide a rich source of examples for multiple and disparate scales. Fluid-mechanical processes are commonly characterized by groups of parameters that are indicative of the various scales in a problem. Some examples are the Mach number (relates velocities to sound speed), the Reynolds number (relates inertial forces to viscous forces), the Prandtl number (relates viscous effects to thermal effects), and the Damköhler number (relates chemical reaction rates to diffusion rates). When any of these numbers is very large (or small) it is likely that the solutions to the models will have regions of localized behavior. For the case of large Mach number the possibility of shocks exists. Similarly for large Reynolds number we expect to encounter boundary layers in the vicinity of solid walls. When the Prandtl number is large we expect that thermal boundary layers will be much thinner than viscous boundary layers. And when Damköhler numbers are large we expect narrow reaction fronts.

In chemical kinetics we find large numbers of chemical reactions competing for the available chemical species at widely different rates. As a result some species are either consumed or produced rapidly or slowly, while other species are being both produced and consumed simultaneously at high rates, with their net production rate being relatively slow. This chemical behavior is responsible for the many widely differing time scales in the mathematical models. The computational models of these processes are characterized as either multirate problems or stiff problems.

It is worthwhile to point out the distinction between multirate problems and stiff problems. In both problems the system itself is equally capable of rapid or slow changes. Multirate problems are those in which at least one component of the solution is changing rapidly, even though others are changing slowly. Numerical methods for these problems must take time steps that are small enough to resolve the fast transients, so they are controlled by accuracy not stability considerations. Stiff problems, on the other hand, are those in which all components of the solution are changing slowly compared with the fastest characteristic scales possible in the model. In these cases explicit numerical methods are forced to take much smaller time steps than are needed to maintain accuracy in order to maintain stability. Often problems that begin as multirate problems become stiff problems as an equilibrium or steady-state condition is approached. Stiff problems are usually solved efficiently by implicit methods.

For stiff or multirate problems, it is perhaps useful to consider methods that treat the fast components differently than the slow components.

Given that multiple-scale problems are of practical importance, we must consider: why are there computational difficulties, and what can be done to ameliorate the difficulties? In the case of disparate length scales one difficulty is that of representing accurately the highly localized behavior. If the solution is represented discretely on a mesh network, the mesh must be sufficiently fine to capture the localized behavior accurately. The whole topic of adaptive meshing is critically important for these problems (see Section 4.2). Here, instead of computing on a fixed prespecified mesh, the mesh adjusts itself dynamically as the solution develops in order to maintain accuracy in the solution.

For situations in which the localized behavior is known to be approximated well by very sharp fronts (e.g., shocks or flames), front tracking methods can have significant advantages. Unlike the adaptive mesh approach where the solution is resolved smoothly through the front, the front tracking methods approximate the front by a discontinuity whose magnitude, speed, and location are to be found. Then elsewhere in the region the conventional discrete representations are adequate.

In problems like chemical kinetics, the disparate time scales cause the governing differential equations to be stiff. Here, explicit solution methods are well known to be extremely inefficient, and some form of implicit method is needed. For systems of ordinary differential equations the problem has been worked out, and high-quality computer software is available. However, when stiffness is encountered in the context of systems of partial differential equations the remedies are much less developed. The same techniques used for ordinary differential equations, when applied directly the partial differential equation problems of practical interest, often yield problems that are simply too large for current computers.

Several approaches show promise. One is to develop operator-splitting methods in which the stiff parts of the problem are split off and solved as a series of smaller and hence more tractable problems. Another approach is to attempt to remove the stiffness by solving instead an approximate (yet sufficiently accurate) system of equations. This tack benefits from an asymptotic analysis of the equations. Both approaches have found recent successes in fluid mechanics and in combustion chemistry.

3.3 SINGULARITIES IN COEFFICIENTS, DATA, OR STATES

Difficulties similar to those encountered in multiple-scale models are often found in problems having singularities in coefficients or states. That is, a singular or discontinuous coefficient can give rise to localized behavior in the solution, such as very steep fronts. An example could be a material interface in a structural or heat-transfer problem, say between a steel and a plastic part. At this material interface the solution (stress or temperature gradient) might change rapidly. In order to maintain accuracy in the computed solution, the numerical procedure would have to resolve this frontlike behavior. The situation is analogous to the occurrence of a shock or a flame front. However, we usually know where the material interfaces are, so they are perhaps easier to deal with than phenomena such as shocks.

Phase transitions can also produce discontinuous coefficients. Take a model in which a melting front is traveling through a region. Usually the properties of the molten material are quite different than those of the solid material. In fact, different governing equations may even be required for the two regions (e.g., fluid motion may be modeled in the liquid but not the solid). In any case, the solution is likely to exhibit jumps in its properties at the transition, and the numerical method will need to locate and resolve it. This situation is more like a shock, in that the position of the phase transition front is not known *a priori*, and thus the numerical method must both locate and resolve it.

3.4 BOUNDARY CONDITIONS

The solution to a boundary or initial-boundary-value problem depends strongly on the boundary conditions. Thus it is important to understand the relationship of the boundary conditions to the differential equations and to their discrete representation. Most important, the boundary conditions must be chosen so that the problem is well posed. For a large class of problems there is a satisfactory theory of admissible boundary conditions, but for many problems, those involving coupled hyperbolic-elliptic systems or disparate time scales, for example, only a rudimentary theory is available.

A possible error in prescribing boundary conditions for hyperbolic equations is to overspecify or underspecify the number of boundary conditions. Overspecification usually causes nonsmooth solutions with mesh oscillations near the boundary. Underspecification does not ensure a unique solution, and the numerical solution may tend to wander in steady-state calculations. In either case, the results are not accurate and one should be skeptical of even the qualitative behavior of the solution. It should be noted that the way in which boundary conditions are specified for the difference equations can change a well-posed continuous problem into an ill-posed (unstable) discrete problem.

Two of the most common methods used to incorporate boundary conditions into discrete equations are the extrapolation and uncentered differences methods. In the extrapolation method, the domain of the problem is extended and the solution is extrapolated to fictitious points outside the integration region. The nonphysical solution at these points is defined so that the discrete equations are consistent with as many relationships as can be derived from the boundary conditions and differential equations. The extrapolation formula can do this best by incorporating the discrete boundary conditions into the extrapolant. Additional relations can be generated by differentiating the boundary conditions with respect to time, replacing all time derivatives by space derivatives using the original differential equation, and discretizing the resulting equations.

The uncentered differences approach is to extend the number of boundary conditions so that all components of the solution are defined at the boundary. Again, these additional boundary conditions must be consistent with the original problem and as many relationships as can be derived from it. An uncentered difference approximation is then used to approximate the spatial derivatives at the mesh points nearest the boundary.

Irregular domains can be imbedded in an underlying regular grid that is not aligned with the boundary, or an irregular grid can be constructed that conforms to the boundary. The discrete approximations to the equations away from the boundary are much simpler on the regular imbedded grids, but the boundary conditions are difficult to approximate. Boundary-fitted grids can be generated algebraically in the original physical domain, or the domain (and hence the grid) can be mapped onto a regular grid in a simpler domain and the equations solved there. The algebraic-grid-generation methods have the advantage that the equations and boundary conditions are unchanged, but the differential operators are more difficult to approximate on the nonuniform grid. When using the mapping method, the differential operations are easily approximated but the transformation can greatly complicate the equation and sometimes obscure important properties such as the conservation laws expressed by the equations.

3.4.1 Boundary Conditions at Infinity

Many physical problems require the solution of partial differential equations on some infinitely large domain Ω. For computational reasons this domain is often replaced by a finite domain Ω_1. Then the difficult problem of specifying boundary conditions at its finite artificial boundary B arises. It is especially important that these artificial boundary conditions do not introduce spurious phenomena. Consider, for example, a nonviscous fluid that at subsonic speed leaves Ω_1 through the boundary B. There is one characteristic direction that points back into the region Ω_1, and therefore one boundary condition has to be specified on B. But, in general, no detailed knowledge of the solution on B is known and therefore other principles have to be applied. For example, if one has solved the problem by difference approximation then one predicts the solution on B from inside ω_1, for all the dependent variables. Thus this procedure amounts to overspecification of the solution on B. Another principle has been proposed, namely, to specify the boundary conditions on B so that no reflection of high frequency takes place. However, numerical experiments have shown that such approaches do not always work.

3.5 BIFURCATIONS AND CHAOS

3.5.1 Buckling and Collapse Behavior, Bifurcations

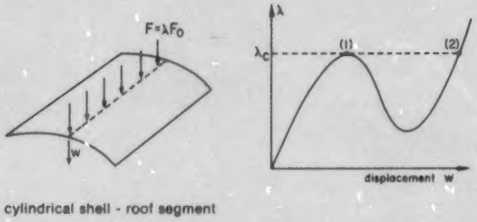
In general, the equilibrium equations of a mechanical structure involve a finite number of parameters, that is, they have the generic form $F(x,p) = 0$, where x varies in some state space X and $p \in R^m$ represents a parameter vector. Thus, in general, the solution set $\{(x,p) \in X \times R^m;\ F(x,p) = 0\}$ is a manifold $X \times R^m$, and one topic of interest is the location and character of the singular points of the solution set.

Without going into detail, suppose that we follow some curve on the solution manifold defined by some combination of parameter values with one degree of freedom represented by a single variable λ. Then we may encounter certain critical points on the solution curve where the mechanical structure may suffer a loss of stability. Such a loss of stability actually corresponds to a dynamic phenomenon whereby the structure undergoes a sudden change of deformation. The dynamics of this phenomenon are not described by the equations of equilibrium $F(x, p) = 0$, but it is possible to deduce from the shape of the (static) solution manifold at that point what type of sudden changes may be expected.

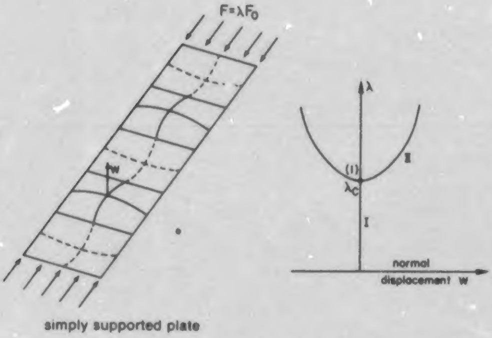
We use a few figures to illustrate the situation. In the upper left-hand part of Fig. 3.1 the point denoted by (1) is a so-called limit point or turning point and an increase of the load-intensity λ beyond the critical value λ_c results in a jump from (1) to (presumably) (2). This type of behavior is called a snap-through or collapse. In the case of the upper right-hand part of Fig. 3.1 the instability phenomenon is related to the bifurcation of the solutions at (1). This behavior is called buckling. This part of the figure is a classical example of stable buckling where a distinct change in the character of the load deformation is encountered when the load-intensity λ passes the buckling load λ_c but where no failure of the structure occurs. On the other hand, the lower part of Fig. 3.1 shows an unstable buckling point where we again observe a dynamic departure from the bifurcation point to some other state [presumably the equilibrium state (2)]. The geometrical shape of the bifurcation branch II is the determining factor in the question of whether the bifurcation point is stable or not.

These examples already indicate that for a deeper understanding of the behavior of a mechanical system it is necessary to analyze the shape of the full solution manifold. Of course, the choice of the parameters entering into the definition of the equation is of critical importance here. In essence, catastrophe theory provides some information about the selection of particular minimal numbers of parameters, but in practice the parameters are simply chosen to correspond to the certain natural features of the structural problems.

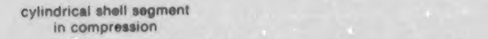
In view of these observations the aim is to develop procedures for a computational analysis of the form of the equilibrium surface. Some methods for this purpose are mentioned in Section 4.4 on continuation methods, but the entire problem is still a wide open research problem. In particular, it has to be noted that we can compute only points that are approximately on the solution manifold of a discretization of the original problem. Thus, the questions arise whether phenomena, such as limit points, or stable or unstable bifurcation points, encountered on the solution set of the discretized problem actually correspond to similar phenomena for the original problem, and, if so, what errors have been encountered. These questions are as yet largely unanswered and represent considerable research challenges. In this connection, it might be mentioned that for nonlinear problems of this type the solution manifold of the discretized equations often has a different number of connected components than that of the original equations. The components that do not approximate the exact solution manifold have been called spurious, or numerically



Collapse Behavior



Stable Buckling



Unstable Buckling

FIGURE 3.1 Instability behavior of shells under different loadings F. On the right the load intensity λ is plotted versus a characteristic deflection W. [From W. Rheinboldt and E. Riks, "A survey of solid techniques for nonlinear finite element equations," *State of the Art Surveys of Finite Element Technology*, Chap. 16, special AMD publ., American Society of Mechanical Engineers, New York (1983).]

irrelevant solutions. They are being observed more and more often in various applications, but their study has only recently begun.

3.5.2 Chaos in Deterministic Systems

It has been remarked that one of the most engaging problems in nonlinear dynamics is that of understanding how simple deterministic equations can yield apparently random solutions. As is now widely recognized, systems with this behavior appear in many of the branches of scientific endeavor. This near universality has come to the attention of physical scientists and applied mathematicians principally through the use of computers in the study of properties of dynamical systems.

The onset of chaos in deterministic systems (the stochastic instability) signals an unusual sensitivity to initial conditions, i.e., the trajectories in phase space diverge widely as time goes on even though the initial conditions are arbitrarily close to one another. The behavior is such as one would expect in a space with everywhere negative Gaussian curvature. On the other hand the trajectories may in fact tend to a single orbit nearly filling a subspace of the phase space (a strange attractor) in an ergodic manner. In even the simplest systems of this type it is possible for several such attractors to coexist side by side, with the initial conditions determining which one is reached asymptotically in time. These and other numerous unusual properties of dynamical systems displaying chaotic behavior have led to some open problems in computational mathematics.

Examples of such problems include the following: When on varying a parameter the stochastic instability sets in, the continued use of an algorithm describing the evolution of the system prior to the onset of chaotic behavior may no longer be appropriate. In this event it may be more practical to take advantage of the stochastic nature of the system and use more or less conventional statistical methods. In order to effect such a change in computational methods it is necessary to detect the change from orderly behavior of the system to chaotic behavior. Theoretically, the sensitivity of the system to initial conditions accompanies the occurrence of positive Lyapounov exponents, i.e., numerical indices of the asymptotic rate of divergence of initially nearby system trajectories. Since the Lyapounov exponents are defined as time asymptotic quantities, straightforward computation of these quantities requires a considerable computational effort, including a calculation of the evolution of two initially nearby trajectories, or the simultaneous integration of the associated variational equations.

An important tool for studying the properties of dynamical systems in the chaotic regime is the first return map, sometimes referred to as the Poincaré map. Such a map displays in a graphical manner various important aspects of the attractor. Unfortunately, the simplicity of generating such a map is restricted to systems no larger than three dimensional, because of the self-evident difficulty of making multidimensional graphic displays. As the study of higher-dimensional dynamical systems advances there will be an ever more urgent need for a higher-dimensional equivalent of the first return map.

As mentioned earlier, in the chaotic regime it may be more appropriate to describe the properties of the system trajectory in statistical terms than in terms of a trajectory evolution. In order to obtain such a statistical description it is necessary to have appropriate information about the invariant measure associated with the given dynamical system. With few exceptions such measures cannot be derived *a priori* but must be obtained from detailed calculations of the trajectories. A finite machine computation of the system trajectory will inevitably introduce some errors that may be all the more serious in the chaotic regime because of the previously mentioned exponential divergence of nearby trajectories. There is then the question of how accurate the computation of a chaotic trajectory must be in order to yield enough information for constructing the appropriate invariant measure.

While the above examples have been drawn from dynamical systems representable by ordinary differential equations there are other systems, e.g., those described by partial differential equations and by integral equations, whose study is likely to be replete with similar computational difficulties.

3.5.3 Symmetry Breaking

Bifurcations commonly arise in connection with a loss, or breaking of symmetry. In such cases the extra structure of the problem symmetry may simplify the analysis. We give an example from fluid mechanics. A classic experiment concerns flow between two rotating vertical cylinders. For small angular velocities of the cylinders the flow is laminar and is called Couette flow. As the angular velocity is increased the vertical translation symmetry is broken and axisymmetric Taylor cells appear. These cells resemble a row of adjacent smoke rings, each one rotating in a sense opposite to its immediate neighbor. A further increase in velocity breaks the axial symmetry, and the Taylor cells become wavy with a time periodic shape. Eventually the flow becomes turbulent. Specific experiments on these systems are a classic topic in fluid mechanics. However as often happens in science, one cannot see important phenomena in the absence of a carefully thought out theory. Recently a number of precise experiments have been conducted concerning the role of strange attractors. Routes to turbulence and, in particular, wavy Taylor cells were carefully observed. The results confirmed some of the theoretical predictions but not all of them. One theoretical proposal was that generic limiting sets, known as strange attractors, would dominate turbulent flow patterns. This proposal was supported by the fact that strange attractors were observed in low-mode approximations to fluid flows. More refined calculations with more modes included indicate an absence of these strange attractors, but the phenomenon is still indicative of the highly complex solution manifolds that can arise in nonlinear problems.

3.6 ILL-POSED INVERSE PROBLEMS

The notion of a well-posed problem is due to Hadamard: a solution must exist, be unique, and depend continuously on the data. The term "data" can have a variety of meanings; in a differential equation it could include any or all of the following: boundary values, initial values, forcing term, and even the coefficients in the differential equation. Since data cannot be known or measured with arbitrary precision, it was felt for a long time that real physical phenomena had to be modeled by mathematically well-posed problems. This attitude has changed considerably in recent years, and it is now recognized that many applied problems are ill-posed, particularly when they require numerical answers in the presence of contamination of the data.

Ill-posed problems often arise in the inversion of well-posed problems. Consider, for instance, a well-posed problem that smooths the data or attenuates its high frequencies. The inverse problem, in which the role of data and solution are interchanged, will then be ill-posed. A simple but important example is the Fredholm integral equation of the first kind

$$\int_0^1 k(x,y)u(y)dy = v(x), \quad 0 < x < 1$$

or, in operator form

$$Ku = v$$

Assuming the kernel to be continuous on the closed unit square, the

Riemann-Lebesgue lemma gives

$$\lim_{n\to\infty}\int_0^1 k(x,y)\sin nydy = 0$$

so that K attenuates high frequencies and thus transforms widely different functions u into approximately the same v. If v is regarded as the data, the solution u of the integral equation, therefore, cannot depend continuously on the data. Indeed, it is not necessarily uniquely solvable, either—take, for example,

$$K(x,y) = \sum_{i=1}^{N} a_i(x)b_i(y)$$

If, unaware of these difficulties, one attempted to solve the integral equation by discretization, one would find that the corresponding matrix problem is singular or ill-conditioned (and the finer the discretization, the more ill-conditioned the matrix problem).

More general inversion problems can also be reduced to an equation of the form $Ku = v$, where K is a continuous transformation, v is the data, and u is the solution being sought. It may happen that u itself is not the quantity of principal interest but rather some functionals of u such as some of its moments or its values at a few specified points.

Thus, there are three pieces of information that are central to the numerical resolution of an inverse problem: (1) the *model* M, representing the equation involving a mapping K between appropriate spaces; (2) the *observation operator* O, representing the measurements that can be made; for instance, we might have $\mathrm{O}(v) = \{v(x_i); i = 1,2,\ldots,n\}$; (3) the *intelligence operator* J, which specifies the information we wish to extract from the solution. For instance, we might have $\mathrm{J}(u) = \{\int x^k u(x)dx;\ k = 0,1,2\}$.

Most of the existing approaches focus almost exclusively on the model M, taking account of *a priori* information about the solution such as smoothness, positivity, and bandwidth. The Tychonov regularization method is of this kind. By restricting K to a suitable subspace it may be possible for the restriction of K to be one to one with a continuous inverse. It might be more appropriate to study the triplet M,O,J for different choices of O and J. One goal of such a new approach would be to classify and quantify ill-posedness by developing comparison principles and order structure.

Ill-posed problems with their attendant numerical difficulties abound in practice. For instance, in scattering from obstacles one may wish to determine the shape of an object (or its surface impedance, if its shape is known) from far-field measurements. Coefficient identification problems arise in many contexts, one such problem being the determination of the sound speed in subsurface media from measurements of the field at or near the surface. Another class of ill-posed problems is associated with image reconstruction (tomography), the medical applications of which are now widely used (CAT scanners, for example) (see Section 2.12). More recently, similar ideas have been applied to the nondestructive testing of mechanical structures to detect cracks in fuel rods, weaknesses in rotor blades of jet engines, and faults in screws in ships. Optimum filtering and inverse problems in Fourier optics (restoring data designed by a band-limited filter, for example) are other areas of current research.

3.7 EFFECTIVE MEDIA

The study of "bulk" or "effective" parameters for composite media is of fundamental importance. Depending on the particular application area it may be relevant to consider a periodic (or an almost periodic) or a random formulation.

3.7.1 Homogenization, the Deterministic Approach

Many problems of physical interest involve several length scales. As an important example we mention the study of composite materials in structural mechanics. Owing to a particular manufacturing process, a distinct structure, e.g., periodically or almost periodicity, is often present.

Homogenization is an approach for deriving the macroscopic properties of the material from the known microscopic ones. A variation of this is to replace a complicated geometrical configuration by a simpler one, e.g., to replace a framework by a plate or to smooth out a rough surface.

Homogenization may be applied to linear and nonlinear problems and can provide qualitative information about physical macrolaws as well as good approximations to the various parameters appearing in these laws.

The most important mathematical tool for the deterministic approach is some form of asymptotic expansion. The theoretical results concern the limiting behavior when certain of the relevant scales become very small.

One is likely to obtain different homogenized formulations from different limiting relations between the length scales.

The numerical solution of a problem introduces a new length scale: the mesh size in a finite-element method, the step size in a finite-difference method, or the wavelength in a spectral method. Different limiting relations between this new length scale and the original physical length scales usually lead to different results. In this sense the numerical treatment has to be considered simultaneously with the homogenization process. One has to design algorithms that will adaptively select the correct homogenized formulation and discretize it appropriately.

Whereas much theoretical work has been done within the last ten years analyzing the effects of multiple scales in continuous media, the study of numerical discretizations of such problems is still very much in its infancy.

3.7.2 Analysis of Random Media

Assessing the effect of random fluctuations in the coefficients of a partial differential equation is a basic mathematical problem that arises constantly in science, applied science, and engineering. Finding effective conductivities of composite conducing materials such as soil or a metal alloy, finding effective fluid equations for flow in porous media (Darcy's law), determining the rate of sedimentation of particles in a fluid, and many other problems are problems that may require analysis of random media. In addition to the quantitative aspects of the problem, many interesting qualitative questions can be posed as well. For example, what is the nature of the spectrum of the Schrödinger equation with a random potential? It has been shown that in one dimension, for a large class of random potentials, the spectrum is always discrete. For randomness of large magnitude, it was recently shown that there is no diffusion, without restriction on the dimension of the space.

From the applications' viewpoint, one can frequently model adequately a random medium, such as a suspension, for example by a continuum with suitable constitutive properties. The continuum equations may be linear or nonlinear, and the constitutive laws may be known only qualitatively from experimental data. In such a context, theoretical investigations are useful and necessary in order to understand how the phenomenological continuum equations arise from the known microscopic structure. One can then find mathematical characterizations for the relevant constitutive laws that can lead to interesting conclusions.

Examples of this arise frequently as, for instance, the determination of bounds for the effective conductivity of composites.

The effective media ideas of Maxwell in the last century dominated theoretical calculations for a long time. In the last two decades, pressing technological needs have caused a major expansion in materials research. In attempting to achieve a mathematical understanding of the methodological basis for effective media calculations that abound, one finds a lack of theoretical foundations.

Mathematical methods in random media are drawn from analysis, probability theory, asymptotic methods, and differential equations. The goal is to develop tools that bridge the gap between microscopic and macroscopic descriptions, give qualitative information about constitutive laws, and determine when residual stochastic effects remain and how they can be characterized. In addition, it is of interest to find important specific problems on which more detailed analysis, including numerical analysis, can be carried out so that these problems can serve as benchmarks in the theoretical development.

3.8 VALIDATION, ERROR ASSESSMENTS, AND SENSITIVITY ANALYSIS

The results look good, but are they really right? The question is often not answered satisfactorily. Indeed, often too little attention is paid to the difficult topic of model and code validation. Once the results look plausible, we are often either unable or unprepared to take the validation process further. The validity of a model depends both on having a proper physical model (Do the governing equations adaquately represent the physics?) and on having an accurate computational representation of the governing equations. The mathematician has a responsibility in both areas. He should help determine the "well-posedness" of the models and from a mathematical point of view help the physical scientist determine the appropriateness of the model. Given that the equations are proper, the computational mathematician must be sure that the numerical procedures used accurately approximate the solutions of the governing equations.

Frequently modeling is done in conjunction with experiments, and those results are used to validate the model. Comparison with experiments simultaneously tests both the validity of the governing equations in the model and of their numerical solution. In this case the source of any discrepancy is not easily isolated. A reasonable goal should be to validate the numerical procedures and the physical models separately so that a model can be developed more confidently. The design of reliable numerical error estimates for the computational methods is an important step.

3.8.1 *A Posteriori* Error Estimates

An important current research topic is the development and application of *a posteriori* error estimates. Such procedures are valuable for models in which differential equations are approximated by their discrete analogs on a mesh network. When *a posteriori* estimates of the error associated with the discretization of the continuous model are possible—and they often are—then potentially it is possible to control the errors. Adaptively moving the mesh network to control or mimimize the error is one application of this approach. With *a posteriori* error estimates, it should be possible, in principle, to give a strict bound for the error on completion of the computation.

The selection of the specific accuracy requirements depends strongly on the goal of the computation. Often it is desired to obtain detailed information about the solution itself; in other cases, the main focus is the value of a specified functional of the solution, as, for example, a stress intensity factor in fracture mechanics or a drag coefficient in fluid dynamics. Other goals may be the determination of certain critical data, such as collapse points or buckling points and their associated loads in structural mechanics. Sometimes special techniques, e.g., variational techniques, can yield highly accurate estimates of particular functionals.

In connection with most of these goals we are interested in quantitative results that have a desired accuracy. For this the error has to be defined, in that a family of exact results has to be specified with which the computed data are to be compared, a norm has to be prescribed in terms of which the error is to be measured, and some procedure has to be established for estimating the error.

Such error estimation capabilities are certainly important in many applications, provided they can be guaranteed to be reliable. For example, for the many types of certification computations required in the design of complex structures or nuclear plants, the availability of reliable estimates of the accuracy of the computed data is obviously important. In other cases, such estimates may reduce the total design effort and avoid unnecessary overdesign. At the same time, the availability of effective error estimates introduces the possibility of applying adaptive techniques to structure the computation to achieve a desired error tolerance at minimal cost or to provide the best possible solution within an allowable cost range.

Many of the theoretical studies of solution algorithms for classes of differential equations provide for some *a priori* error estimates, usually of an asymptotic type. For the practical error assessment these *a priori* bounds are rarely computable or very accurate. Thus, one is led to the necessity of developing *a posteriori* error estimates that utilize information gained during the computation itself.

For the finite-element solution of certain classes of elliptic boundary-value problems, some computable and reliable *a posteriori* error estimates have been developed and analyzed in recent years. Most of these *a posteriori* estimates are based on a local analysis. For a given mesh Δ consisting of elements $\Delta_1, \ldots, \Delta_n$ and with a corresponding approximate solution on that mesh, an error indicator η_j is associated with the jth element Δ_j. These η_j have to be computable in terms of information about the problem and the approximate solution on Δ_j and, at most, on the immediate neighbors of that element. On the basis of the indicators $\eta_1, \ldots, \eta_n$ an error estimate $\epsilon(\Delta)$ is then constructed. Of course, the η_j as well as $\epsilon(\Delta)$ depend on the chosen norm. The theoretically important question is then the relationship between $\epsilon(\Delta)$ and the norm of the actual error $e(\Delta)$. The effectivity of the estimation may be judged by the effectivity index $\theta = \epsilon(\Delta)/||e(\Delta)||$. In practice, it is usually more important for θ to be close to 1 than that $\theta \leq 1$. Moreover, it is essential that θ converges to 1 when $||e(\Delta)||$ tends to zero, so that for an accuracy of, say, 5 to 10 percent the value of $|\theta - 1|$ is expected to be less than, say, 0.1 or 0.2.

The requirement of designing error estimators with these properties for realistic classes of problems and various different norms certainly represents a demanding research task. The results available so far suggest that such error estimators can be developed at least for linear problems. For nonlinear problems the situation is in an embryonic stage although some results available for model problems in one space dimension indicate that estimators for the error along continuation paths and for the location of critical points are computationally feasible. There is certainly considerable need for concentrated research in the general area.

3.8.2 Other Validation Measures

Checking for mesh dependencies and convergence rates is another way to help validate a model. If a method is supposed to be, say, "second order," then as the mesh intervals are halved, the errors should be reduced by a factor of 4. If this does not happen according to one's error estimate, then the method does not have the desired order yet and may be in error. Also one should continue to refine the mesh until the results are independent of refinement to within the desired accuracy. Solutions can also be checked for sensitivity to mesh orientation. The solution should not be aligning itself with some special property of the mesh network.

Numerical methods can also be validated by comparing them with analytic solutions. Often this is possible by choosing limiting cases where an asymptotic analysis applies. In some cases complex constitutive laws can be replaced with constants so an exact solution is possible. Higher-dimensional models can sometimes be validated by comparison with previously confirmed lower-dimensional results. Bounds on solutions are another way to help verify a model. Often conservation laws or minimum and maximum principles apply, or the solution is known to approach a previously known equilibrium or steady-state condition. These properties can be used as a basis for validation.

To the extent possible one should always write computer codes in a modular fashion such that each part of the model can be validated separately. Even though this is just good structured programming practice, and not necessarily related to mathematics, it is an important aspect of model validation.

3.8.3 Sensitivity Analysis

In addition to the independent and dependent variables, most models also depend on certain physical parameters. Unfortunately, those parameters are often not known accurately. Sensitivity analysis is a systematic means to quantify the relationship of model parameters and model results. Doing the sensitivity analysis requires solution of an additional system of differential equations. These equations are a formal statement of the relationship between the dependent variables of the system and the parameters. The results are given in terms of a matrix of partial derivatives of the dependent variables with respect to the system parameters. One way to think of the analysis is as a method to provide theoretical "error bars" for the model.

New methods are being developed to solve these sensitivity equations quite efficiently. The methods rely on the observation that the sensitivity equations are linear, regardless of the nonlinearities in the original model. The method solves differential equations for the Green's function of the sensitivity equations, and then the sensitivity coefficient matrices are computed by quadrature for the various imhomogenous terms corresponding to the parameters. These methods have been successfully applied to problems in chemical kinetics.

4. NUMERICAL METHODS

4.1 DISCRETIZATION METHODS

Many important physical problems are modeled by boundary or initial-boundary-value problems. In this modeling, the physical state under consideration is characterized by a function u, which is the unique solution to the boundary or initial-boundary-value problem. Thus a major part of the analysis of the physical problem is the determination of u or some of its derivatives or some functional of it.

In nearly all important problems the determination of u is an infinite-dimensional problem in the sense that u does not lie in an explicitly known finite-dimensional space or, alternatively, cannot be expressed in terms of a set of explicitly known functions by means of a finite set of parameters. Thus u, cannot be "completely" represented on a computer, and it is necessary to resort to some type of approximation or discretization method. In essentially all discretization methods one attempts to construct a function, $u_{\mathbf{approx}}$, which on the one hand is "close" to u and on the other is characterized by a finite set of parameters, and so can be calculated.

The aim of finding $u_{\mathbf{approx}}$ that is "close" to u is made precise by requiring that $||u - u_{\mathbf{approx}}|| \leq \tau$ (or that $||u - u_{\mathbf{approx}}|| \leq \tau||u||$), where $||\bullet||$ is a physically relevant norm and τ is a physically relevant tolerance. The goal is thus to find $u_{\mathbf{approx}}$ satisfying this error criterion with the least expenditure of computational effort. The selection of a discretization procedure is influenced by a number of considerations, the most important of which we now list:

1. The goals of the analysis of the physical problem.
2. Known mathematical properties of the physical problem and the algorithm.
3. Hardware considerations, e.g., the availability of parallel processing.
4. Computer-science considerations, e.g., data-management requirements.
5. Restrictions on computation time and expense.

74

As indicated above, the exact solution is approximated by a function u_{approx}, which is expressible in terms of a set of explicitly known (basis) functions by means of a finite set of parameters, which are determined in the computation. One broad classification of methods is in terms of the nature of the basis functions, namely (a) those involving global basis functions having global support and (b) those involving local basis functions having small support. Another classification is based on the extent to which the method is adaptive. Adaptive methods refine and modify themselves on the basis of partially completed computations.

Of course, these classifications are not precise, and there are methods possessing the different properties in various degrees. We now turn to a more detailed discussion of the most commonly used discretization procedures.

4.1.1 Finite Differences

One of the most frequently used discretization methods is the method of finite differences. The central idea is to replace each partial derivative occurring in the differential equation in the underlying boundary or initial-boundary-value problem by an approximating difference quotient. For example, the first-order derivative $\partial u(x,y)/\partial x$ may be replaced by the forward difference $[u(x+h,y)-u(x,y)]/h$ or the backward difference $[u(x,y)-u(x-h,y)]/h$, whereas the Laplacian $\Delta u = u_{xx}+u_{yy}$ may be replaced by the five-point difference operator

$$\Delta u \approx \frac{u(x+h,y)+u(x,y+h)+u(x-h,y)+u(x,y-h)-4u(x,y)}{h^2}$$

This replacement of all derivatives in the differential equation by appropriate difference quotients leads to a system of equations, called difference equations, for the numbers u_{ij}, which are to approximate the values of the exact solution $u(x,y)$ at the finite-difference mesh points (jh,kh), $j,k=0,\pm 1,\pm 2,\ldots$, where h is a small positive number, called the mesh parameter. Nonuniform meshes may be considered as well, but at considerable complication in the form of the difference quotients in the resulting difference equations.

There are a number of important questions that arise in connection with the study of difference methods, namely questions of

1. Accuracy of the method;
2. Stability of the method;
3. Efficient solvability of the finite-difference equations;
4. Robustness of the method with respect to the input data (e.g., coefficients, forcing functions, meshes); and
5. For nonlinear problems, the separation of legitimate approximate solutions, which correspond to an exact solution, from spurious approximate solutions, which do not correspond to any exact solution.

Finite-difference methods are an example of the local basis class of approximation methods. They can be adaptive. Adaptivity is usually introduced via adaptive mesh selection: the mesh chosen at any stage in the computation is based on the previous computations.

Much important work on difference methods remains to be done. We mention in particular the construction of effective difference methods for nonlinear problems, in particular for those problems whose solutions have shocks.

4.1.2 Variational Methods of Discretization

We will now discuss a class of discretization methods based on variational formulations of the physical problem under consideration. As noted above, the problem of calculating the exact solution u is infinite dimensional in the sense that u is only known *a priori* to lie in an infinite dimensional space, say H. For a linear problem, a variational method of discretization consists of (a) a finite-dimensional space $S \subset H$, called the trial space, in which the approximate solution is sought, (b) a finite dimensional test space V, and (c) a bilinear form $B(u, v)$ defined on $H \times V$. The approximate solution is then determined by requiring that

$$u_{\mathbf{approx}} \in S$$

$$B(u_{\mathbf{approx}}, v) = B(u, v), \quad \text{for all } v \in V$$

where for $v \in V$, $B(u, v)$ is computable from the data of the problem without knowing u. Since S and V are finite dimensional, $u_{\mathbf{approx}}$ can be calculated by means of the solution of a system of linear equations if the original equation is linear. Usually, for nonlinear problems, B is nonlinear in u, and the resulting system of equations becomes nonlinear.

The approximate solution depends on the selection of S, V, and B. For any problem there exists a wide variety of variational methods of discretization, i.e., a wide variety of choices for S, V, and B. The rational selection of S, V, and B is a central problem.

Variational methods can be of either the local-basis or global-basis type. Of those of global-basis type we mention the various versions of the spectral method and the p version of the finite-element method. Finite-element methods, considered in more detail below, and collocation methods are typically of the local-basis type. We also note that variational methods can be adaptive.

4.1.3 Finite-Element Methods

Finite-element methods arise if for S and V we choose spaces S_h and V_h of piecewise polynomials of fixed degree. That is to say, the underlying spatial domain for the problem is broken up into small geometric pieces, called "elements," whose size is measured by a parameter h. The functions in both S_h and V_h are then restricted to be polynomials in x and y on each piece but allowed to be different polynomials on the different pieces. In designing finite-element methods, i.e., in selecting S_h, V_h, and B, one attempts to achieve approximability, stability, and systems of equations that can be solved effectively.

Approximability here refers to the ability of the space S_h to approximate the unknown solution u. The solution u is unknown *a priori*, and often only the information $u \in H$ is available. In such situations S_h has to be selected so that every function in H can be approximated sufficiently well by one in S_h. However, an approximation based on a few large elements can provide additional information on u, which can be used in turn to refine those elements. This type of adaptive element selection is especially important for problems with sharply varying solutions (see Section 4.2).

In the choice of the bilinear form B one has, in effect, the freedom to choose a variety of variational principles, many of which have a natural physical connection with the original problem. For instance, the standard Ritz method is based on the principle of minimum potential energy. An alternate variational principle is the complementary energy principle. Approximation methods based on this principle are referred to as complementary energy or equilibribum methods. These methods involve a constraint that is usually difficult to satisfy. One way to circumvent this difficulty is to treat the constraint by means of a Lagrange multiplier. This leads to the so-called mixed methods. They appear to be promising for many important problems and have recently received a large amount of attention.

4.1.4 Transformation Methods

In the transformation or pseudospectral method, the discrete approximation u is first mapped by a transformation of the form

$$Tu = \sum_{j=1}^{m} a_j \phi_j(x)$$

into the m-dimensional function space of the coefficients, a_j. The basis functions ϕ_j and the transformation are chosen so that T and T^{-1} are fast (order of $m \log m$ operations) and so that differentiation D is simple in transform space. The derivative approximation can then be written as

$$\frac{\partial u}{\partial x} = T^{-1} D T u$$

Some common transforms are based on the fast Fourier transform, where the ϕ_j are trigonometric functions or Chebyshev or Legendre polynomials. Selecting the ϕ_j as piecewise polynomials with compact support, such as the B-splines, is another good choice. By choosing the transformation to incorporate some crucial property such as the periodicity or symmetry of u one can improve the accuracy of the method for a fixed number of basis functions. This can sometimes best be done by choosing the basis functions close to the eigenfunctions of the differential equation.

4.1.5 Semidiscrete Methods

When solving a partial differential equation one sometimes discretizes with respect to some but not all of the variables. For example, for the diffusion equation governing the cooling of a hot rod, one may discretize with respect to the space but not the time variable, thereby replacing the original partial differential equation by a system of ordinary differential equations. Such an approximation method is referred to as a semidiscrete method or as the method of lines. Semidiscrete methods may be used for hyperbolic as well as parabolic equations.

One has, of course, eventually to discretize with respect to the time variable as well. Semidiscrete methods are based essentially on the view that very effective time discretization methods are available (in the form of preprogrammed software packages for the solution of ordinary differential equations) and that the spatial discretization is the main concern. An alternative point of view is to consider both discretizations simultaneously. Such fully discrete methods have been analyzed and tested extensively.

Among important research problems for semidiscrete methods we mention the problem of adaptive mesh selection for the spatial discretization.

4.1.6 Method of Characteristics

This is a method for hyperbolic equations, particularly for those involving only one space dimension. In these equations the solution at some point in space-time depends primarily on its values along a fixed, finite number of curves (characteristics) going back in time from the given point. The approximations to these values are determined from difference equations that are closely related to the characteristics of the differential equations. This method has a natural generalization to quasi-linear second-order equations in two independent variables. It is especially important for problems whose solutions have shocks.

4.2 ADAPTIVE GRID METHODS

For realistic problems it is rarely feasible to design numerical processes that are reliable and accurate at a reasonable cost and yet that do not utilize some form of adaptivity. Put simply, most two-dimensional and virtually all three-dimensional problems are undercomputed without this technique. This statement will almost certainly remain true after the next generation of computers is available. The adaptive approach is to distribute the computational effort nonuniformly, so as to concentrate on the most singular parts of the solution or the most important parts of the solution from the point of view of critical design parameters. Correspondingly, one must give less computational effort to the regular or less critical parts of the solution (also see Section 4.9). At the same time, adaptive approaches may also lead to a simplification of the input data needed for the program and hence free the user of part of the drudgery typical in preparing such input and in having to make the many *a priori* decisions required by most of today's programs.

The goal of adaptive grid methods is to choose a grid that is particularly refined, or that is aligned or oriented optimally, with respect to the solution in regions of space and time that are critical for solution accuracy. Thus adaptive grids utilize local mesh refinement or optimal local mesh orientation.

The simplest adaptive grid is a preliminary, analytically determined coordinate transformation. For example, in the transformed coordinates the problem may be approximately independent of one variable or otherwise simplified. The next strategy is to choose a numerically determined coordinate transformation. Typically, in two dimensions the coordinate transformation is obtained by the solution of a subsidiary partial differential equation. The resulting grids may be expected to give both improved mesh refinement and mesh orientation. The method is somewhat problem dependent and can give rise to discretization errors in the mapping of solution variables between the various grids.

Lagrangian grids for time-dependent problems are adaptive for material interface singularities, because the grid points move with the material particles. Since these well-established methods also develop rezoning and mesh entanglement problems, they provide a reservoir of experience concerning the difficulties associated with other evolving, adaptive algorithms.

A refined grid can be constructed without recourse to a coordinate transformation. In response to a critical solution parameter or solution error criteria, selected regions of space can be flagged, preferred orientations selected, and refined subgrids introduced locally. Then, small time steps are chosen on the finer subgrid, and an interpolation problem must be solved to blend fine and coarse grid solution values. Finally, the construction is recursive, so that three, four, etc. levels of refinement can be introduced automatically, in response to some *a posteriori* error estimate on the next coarser grid. Precisely defined, reliable error estimators appear to be central to the design of effective adaptive procedures.

In the context of finite elements for elliptic problems there is a developed theory for *a posteriori* error estimates (and, hence, for adaptivity), which is based on local analysis. For a given mesh made up of elements $\Delta_1, \ldots, \Delta_n$ and with the aid of the corresponding approximate solution, an error indicator η_j is computed for each element Δ_j. For certain classes of problems it has been proven that asymptotically the errors become optimal when all the η_j become equal. This equilibration principle provides the basis for the control of the adaptive process. In essence only those elements

Δ_j are refined for which the error indicators are too large in comparison with those of the other elements. And elements that are unnecessarily small are combined with their neighbors. The study of suitable algorithms for this has only recently begun. For example, some results have been obtained for algorithms based on the assumption that during the refinement process none of the elements could be combined without increasing the maximum value of the error indicators.

In time-dependent problems, differential equations can be introduced for the ever-changing optimal location of the grid nodes. These equations are then solved simultaneously with the original partial differential equation, leading to what are known as moving mesh methods.

Alignment of the grid without refinement is also possible, if fixed or moving boundaries or interior interfaces are specified as part of the problem. By alignment (without refinement), a regular grid index structure can be preserved. Maintaining the grid structure has the advantage that it potentially allows fast iterative methods, such as fast Fourier transforms, to be used as part of the solution algorithm.

Adaptive grid techniques have been applied successfully to a range of time-independent problems. The newer time-dependent methods need to be developed to the point where they can be applied to meaningful two- and especially three-dimensional problems and compared with alternative methods. An important question requiring further attention is the construction of efficient, computable *a posteriori* error estimates for realistic classes of problems. Specifically, even for steady-state problems, there is the question of the validity of the equilibration principle mentioned above as well as the design and analysis of suitable adaptive control laws to implement this principle. This latter problem may require examination and incorporation of results in such fields as automatic control theory, artificial intelligence, and learning processes. It also raises the problem of the choice of appropriate refinement techniques that produce meshes with desirable properties. Last but not least there is the question of data management, which must be handled successfully to control the vastly increased algorithmic complexity associated with adaptivity and to achieve computational efficiency.

4.3 METHODS FOR SOLVING DISCRETIZED DIFFERENTIAL EQUATIONS

Finite-difference and finite-element discretizations of partial differential equations usually give rise to large systems of equations in which each unknown is coupled to only a few of the other unknowns. Systems with tens or hundreds of thousands of equations are relatively common. For time-dependent problems these systems arise from the use of implicit time discretizations. For sufficiently fine grids, the numerical solution of these systems consumes a major part of the computer time for an entire simulation.

Most nonlinear systems are solved by some form of iterative method based on linearization, such as Newton's method. At each step, these methods result in large sparse linear systems. In many cases, iterative methods converge only if the initial guess is sufficiently close to the solution.

There are two basic approaches to solving large sparse linear systems of equations: direct sparse matrix methods (i.e., some form of Gaussian elimination that takes advantage of the location of most of the zeros) and iterative methods, where the sparsity makes each iteration relatively inexpensive. No method is best for all problems. For many problems a combination of methods is attractive. Usually this takes the form of a block iterative scheme using a direct method to solve the subsystems whose diagonal blocks are matrices. Combination methods are of particular importance for the solution of linear systems arising from coupled systems of partial differential equations.

Direct methods are relatively well understood today, and a number of excellent implementations of them exist for serial computers. Direct methods vary in the extent to which they take zeros into account. The simplest, nontrivial approach is band elimination, which takes account only of those zeros occurring outside the band determined by the extreme nonzeros of the matrix. The most complex approach is general sparse elimination in which all the entries that remain zero during the elimination are taken into account. For systems that do not require pivoting (e.g., those having symmetric, positive definite matrices) there is a symbolic preprocessing phase in which the location of these zero entries is calculated. There exist good techniques (the nested dissection ordering and the minimum degree ordering) for arranging the unknowns and the equations so as to minimize the zero fill-in during elimination. For model problems it has been shown that the nested dissection ordering provides asymptotically optimal results with respect to work and storage. The minimum degree algorithm is a valuable heuristic approach that is competitive in practice but that has defied analysis. For systems that require pivoting for numerical stability one cannot compute the zero structure *a priori*. Moreover, the ordering of the unknowns and equations to minimize zero fill-in will usually be significantly altered.

Some of the strong points of direct methods are as follows: (1) They provide an exact answer (modulo round-off error) to the linear system with a fixed number of operations independent of the system's condition number. Most production structural analysis packages such as NASTRAN use some form of direct method, even for three-dimensional problems. In these applications (many of which are based on fourth-order elliptic problems) it is necessary to use higher-order precision because of conditioning problems. (2) For problems with two dependent spatial variables, their execution time is often shorter than the execution time for iterative methods, especially for problems of moderate size. Some of their principal disadvantages are the following: (1) they require considerably more storage than iterative methods, even for two dimensions; (2) they will almost always be noncompetitive with iterative methods for three-dimensional problems in terms of running time; and (3) except for the simpler methods such as band elimination (and to a lesser extent profile or envelope elimination) they do not vectorize well. In fact, owing to the necessary indirect addressing involved, there are as yet no efficient implementations of general sparse direct matrix methods for the CRAY-1 or CDC CYBER-205 supercomputers.

Except for structural problems, iterative methods are commonly used. Classical iterative methods, such as successive overrelaxation, Chebyshev semi-iterative methods, and such newer methods as the preconditioned conjugate gradient method, are fairly well understood for symmetric, positive definite systems, and they are easy to implement. However, the situation is not so bright for nonsymmetric or indefinite systems, though in practice classical iterative methods may converge rapidly with a clever choice of the iteration parameters. Nonsymmetric systems with indefinite symmetric parts are especially difficult to solve, and no satisfactory general algorithms are known at this time. Such problems arise in the simulation of secondary and tertiary thermal recovery techniques for petroleum reservoirs (see Section 2.6).

Some of the principal advantages of iterative methods are the following:

1. They tend to require minimal storage (proportional to the number of unknowns);

2. They are reasonably fast for a wide range of problems. Moreover, the number of iterations required is independent of the number of space dimensions in the underlying partial differential equation (but not of their order, or of the mesh size);

3. They can take advantage of good initial guesses to the solution, as would be available in time-dependent or nonlinear problems; and

4. Many of them vectorize reasonably well on supercomputers.

Some of their disadvantages follow:

1. Mathematically rigorous stopping criteria may be difficult to formulate, e.g., for linear systems with matrices that are not symmetric, positive definite;

2. Many of the methods require a selection of iteration parameters, and the performance of the methods depends critically on such a selection (this difficulty is being overcome somewhat by the relatively new adaptive methods and the preconditioned conjugate gradient-type methods);

3. The interaction between linearization and iteration is not well understood, especially for discretizations of coupled systems of partial differential equations; and

4. Nonsymmetric or indefinite problems may cause great difficulties for iterative methods.

The relatively new multigrid iterative method combines the well-understood behavior of a given iterative technique with the fact that an underlying differential equation is being solved approximately. It alternates iterating, toward the differential equation's solution, on fine and coarser subgrids of the spatial network, with the goal of performing no more computational work on the finer (hence expensive) grids than is absolutely necessary. In many cases of practical interest, such as in neutron diffusion in complex environments, the technique yields sufficiently accurate solutions to the equations in a computational time proportional to the number of unknowns. This has been a long-sought-for goal in the approximation of elliptic equations in more than one space dimension. As an iterative method it also has a natural extension to nonlinear equations; and its logical structure, together with the already necessary calculation of residual errors, points toward the incorporation of adaptivity for the nesting spatial grids.

4.4 CONTINUATION AND HOMOTOPY METHODS

For more than a century the so-called continuation principle has proved to be an important tool in mathematical theory. For example, early uses date back at least 100 years to H. A. Schwarz and his work on conformal mappings; then, in the early part of this century, J. Hadamard and M. Levy applied these techniques in connection with the inversion of nonlinear mappings, and it is also a basic tool in J. Leray and J. Schauder's work on differential equations. But it was essentially only in the early 1950s, with the advent of automatic computing, that continuation approaches began to be used in numerical applications. Since then they have grown into an extremely powerful technique for the numerical solution of wide classes of nonlinear problems.

One of the problems to which continuation techniques are applied concerns the solution of a nonlinear equation $F(x) = 0$ in some space X. In order to compute a specific solution $x^* \in X$ a possible approach is to imbed the equation into a family of equations $H(x,t) = 0$, $0 \leq t \leq 1$, for which there exists a computable solution path $x = x(t)$, $0 \leq t \leq 1$, in X beginning at a known point $x(0)$ and ending at the desired solution $x(1) = x^*$. In other words, one considers a family of smoothly changing problems, the final problem being the original problem in question and the initial problem being one whose solution is easily determined. Use of the continuation, therefore, requires an ability to solve a sequence of problems when the solutions to nearby problems are known.

A related, but conceptually distinct, problem arises in many applications in science and engineering where the equation under consideration always includes a number of physically relevant, intrinsic parameters. In other words, the equation has the generic form $F(x,p) = 0$, where x belongs to some state space X and p varies in a parameter space P. In this setting it is rarely of interest to determine only a few specific solutions. Instead, the requirement is to follow paths on the solution manifold $\{(x,p) \in X \times P;\ F(x,p) = 0\}$ in the space $X \times P$ of all state and parameter variables and thereby to detect specific features of the manifold that signify a change of behavior of the system under study.

For the first of these problems, namely the computation of a specific solution of some question, two distinct continuation techniques are available. The first involves the case when the path of solutions to the family is smooth, which in turn allows its representation as a solution of a differential equation. The second approach is based on homological rather than homotopic concepts and makes use of a numerical form of a result in algebraic topology (Sperner's lemma). This approach has been reformulated and is now considered principally in the form of algorithms involving piecewise-linear solution paths. Much of the recent research in this area concerns these piecewise-linear continuation methods and their application to fixed-point problems in economics optimization and game theory.

Continuation methods for following paths on the solution-manifold of parametrized equations developed mainly in structural engineering under the name of incremental methods. Applications to other areas, as, for example, to computational fluid dynamics and to phase transitions in statistical physics have only begun to appear relatively recently. For a numerical analysis of a given solution, manifold continuation methods have to be considered in a broader sense as a collection of numerical procedures for completing a variety of tasks, including the following:

1. Follow numerically any curve on the manifold specified by an *a priori* given combination of parameter values with one degree of freedom.
2. On any such curve determine the exact location of target points where a given state variable has a specified value.
3. If desired, at any such target point switch to the trace of a different solution path;
4. On any such curve identify and compute the initial points where stability may be lost;
5. From any one of the critical points follow a path in the critical boundary. In contrast to the case under 1, such paths are typically specified by combinations of the parameters with two degrees of freedom together with the implicit requirement that all points of the path are in the critical boundary.
6. On any solution path determine the location of bifurcation points and the paths intersecting at that point.

For specific applications additional tasks may arise. For instance, if the parametrized equation represents the equilibrium equation of a system of differential equations then we may wish to locate Hopf bifurcation points on a particular solution path where periodic solutions of the dynamical system branch off from the static equilibrium.

In recent years much research has been devoted to these various tasks, but there remain many open questions especially in connection with the more specialized tasks, such as the location of Hopf bifurcation points. Moreover, library-quality packages for the basic tasks 1-3 are still under development, and the software is by far not so advanced as, say, in the case of software for the solution of ordinary differential equations. For specific applications, as, for example, to fluid-dynamic problems or to the case of structural problems involving plasticity, creep, and viscoelastic effects, the situation is still wide open; and only relatively *ad hoc* techniques are available.

4.5 OPTIMIZATION METHODS

Optimization problems occur in all areas of science, engineering, economics, and applied statistics. They may involve some least-squares approximation of observed data, fitting of parameters occurring in a mathematical model on the basis of experimental observations, optimization of the design of an engineering structure, optimal control of an engineering system, or modeling of economic or business systems. These are only a few examples that do not even begin to cover the numerous types of optimization problems that arise in practice.

Broadly speaking, in all of these problems a real function, usually called the objective function, is to be minimized or maximized over some constraint set in a given finite- or infinite-dimensional space. The problems differ considerably depending on the mathematical characteristics of the objective function and the constraints, the dimension of the space, the amount of computable information that is available, and the requirements of specific applications.

A good overview of the research problems concerning computational methods for such optimization problems in finite-dimensional spaces has been given in the report *Program Directions for Computational Mathematics*, June 1979, prepared for the Applied Mathematical Sciences Research Program of the U.S. Department of Energy (edited by R. E. Huddleston, Sandia National Laboratories). This report identified the following research areas:

1. Analysis and comparison of techniques for dealing with nonlinear inequality constraints.
2. Construction of algorithms for environments where computer storage is restricted.
3. Production of high-quality software and other software-directed activities.
4. Development of algorithms and software for problems in which some of the variables are discrete or integer.

5. Techniques to assist in finding global (or specified) minima.

6. Large-scale linear programs with special structure, e.g., staircase and block-angular.

7. Methods for nondifferentiable optimization.

8. Techniques for selected nonlinear estimation problems, such as separable or constrained least squares, and data fitting in special norms.

9. Investigation of the connection between fixed-point methods and alternative methods for solving nonlinear equations.

10. Further study of selected aspects of linear constrained problems, such as special types of constraints, application of conjugate gradient techniques, the merits of various active set strategies, and the influence or scaling.

The report does not address infinite-dimensional problems, for example, problems in control theory or the calculus of variations. Here the mathematical problems often become formidable, and special techniques are needed in most applications. For the computational solution, the principal approach applies finite-dimensional optimization methods to a discretized form of the problem. This, in turn, raises the usual questions concerning the convergence and quality of the approximations.

4.6 GRAPH-THEORETICAL METHODS

Many physical systems, or their mathematical models, involve a number of discrete objects that are the producers or users of certain data or commodities and that in turn are interconnected by links that can transmit these items from one of the objects to another one. The underlying mathematical structure is then a graph consisting of a collection of vertices connected by arcs or branches.

The modeling of some classes of physical systems in terms of graphs is rather natural, for example, in the case of communication or transportation networks where the branches represent, say, power lines, roads, airline routes, or water pipes, and, correspondingly, the vertices are power-generation stations, communities, airline terminals, or water reservoirs. In other cases the connection between a particular problem and its graph-theoretical interpretation is less obvious, for example, in the case of a discretization of a particular boundary-value problem on a given grid or the representation of a collection of data in a computer.

Corresponding to the wide range of applications, the forms of graph problems differ widely. For certain network models interest may center on the connectivity properties of the graph, that is, on the determination of whether a particular commodity can be transported between specific vertices. Then questions arise about the maximum possible flow that can be accommodated under particular constraints. These problems in turn are related to the so-called vulnerability and reliability problems for networks. On the other hand, if time enters into consideration then questions of waiting time and of best routing may arise. These are only a few of many types of such problems.

From a computational viewpoint these various problems have stimulated the development of numerous combinatorial and graph-theoretical algorithms. But there remain many open research questions, especially when it comes to the production of general, robust software and the availability of algorithms for problems involving large graphs.

Graph-theoretical formulations are also finding increasing application in connection with the numerical solution of problems that do not have an inherent graph-structure. One such class of problems concerns the computational handling of large sparse matrices. Many of the algorithms used here perform a sequence of steps that transform the matrix into successively simpler matrices of, say, a more nearly upper triangular or diagonal type. These transformations achieve their aim by introducing zeros in place of originally nonzero matrix elements. But, as an unavoidable byproduct they also introduce nonzero elements in places where the original matrix elements were zero. Thus, in order to exploit the sparsity structure of the matrix one must provide a data structure that either allocates from the outset space for all the fill-in during the computation or that allows for a dynamical allocation of space for the fill-in when it occurs. In both cases, graph-theoretical approaches form the basis for the design of desirable algorithms.

An example of the use of a static data structure is the case when a row and column representation can bring the matrix into banded form with small bandwidth. This is frequently the case of the linear systems arising in the finite-element discretization of elliptic boundary-value problems, and the corresponding bandwidth optimization routines are widely used in practice. On the other hand, if a dynamic storage structure is used, then special care has to be taken in the design of pivoting strategies for reducing fill-in while at the same time maintaining numerical stability. Various sparse matrix packages have been developed for this purpose. They are typcially rather large and complex pieces of software. But the field is still under active development, and there remain many open research questions.

In particular, much still needs to be done on the interrelation between sparse matrix algorithms and special-purpose computer architectures.

In recent years graph-theoretical approaches have also found increasing application in the design of algorithms for the numerical solution of problems of mathematical physics, in particular, of fluid dynamics. For example, it has been observed that certain natural finite-difference discretizations of the equations of viscous, incompressible flow admit interpretations as systems defining flows on certain associated networks. Typically, the network nodes correspond to the idealized control volumes represented by the mesh points of the finite-difference equations, whereas the network arcs correspond to the paths on which one may identify the discrete finite-difference mass fluxes. Such observations can lead to remarkable savings in computing costs because they open the way to *a priori* transformations of the original (discretized) system of equations to completely equivalent systems in substantially fewer variables. For flow problems in two and three space dimensions the reduction factors are nominally 1/3 and 1/2, respectively. In graph-theoretical terms this approach corresponds to the transformation of the Maxwell-node equations to the Maxwell-mesh equations, long used in electrical-circuit problems.

The key requirement in the application of network techniques to fluid-flow problems is that the discretized momentum and continuity equations be interpretable as "Ohm's laws" and "Kirchhoff-node laws" on an associated network. This requirement permits great generality in the actual form of these laws and easily accommodates both implicit time-dependent as well as nonlinear steady-state difference forms of the Navier-Stokes equations.

It is even possible to extend the network approach to compressible flow problems. Here the new idea appears to be the introduction of pseudo-flows into the node law and the identification of corresponding pseudo-characteristics to augment the Ohm's laws obtained from the momentum equations. In the nonstationary case, this produces numerical schemes whose stability is independent of local acoustic velocities.

The entire area is still under active research development. For example, there are efforts to bring multispecies flow problems under the purview of network theory. This includes, as an important special case, two-phase flow problems that are a central concern in the design of reliable energy-generating systems and the safety analysis of nuclear power plants.

4.7 SPLITTING METHODS AND DEFECT CORRECTIONS

Splitting is a means to separate a large intractable problem into a sequence of smaller, or at least more easily solved, problems. These methods are invoked to reduce significantly the computational effort (time and memory) needed to solve a problem compared with solving it directly. Often a form of splitting is required to make solution practical, and some cases even tractable. Various forms of splitting are common in engineering and scientific applications, even if they are not always recognized as such.

Defect correction is a widely used, if often unlabeled technique of splitting. It presumes that one wants to solve a given hard problem, that one has in hand a guess at its solution, and that one also has a nearby problem that can be solved easily. It corrects the guess by solving the easier problem with special data computed from the guess.

To illustrate the method, suppose that after discretization it is necessary to solve a finite-dimensional system of equations of the form

$$A(v) - b = 0$$

where A is a nonlinear operator, b is a known vector, and v is the solution. Often v is difficult to obtain directly, but the residual error

$$r = A(w) - b$$

for an approximate solution w is easy to evaluate. If there is a related system

$$P(w) - b = 0$$

that approximates the original system and that is easier to solve, the defect correction algorithm may be appropriate. Given an estimate v_n near a root v_{n+1} of the original system, we can expand the original equation in a Taylor series to get

$$0 = A(v_n) - b + P(v_{n+1}) - P(v_n) - (J_P - J_A)(v_{n+1} - v_n) + O(\epsilon^2)$$

where $\epsilon = v_{n+1} - v_n$. The defect correction iteration is any approximation to the above equation. The simplest such iteration is

$$P(v_{n+1}) = P(v_n) - A(v_n) + b$$

This iteration will converge if v_n and J_P (the Jacobian of P) are near enough to v_{n+1} and J_A, respectively.

One of the most common splitting algorithms in engineering applications is the alternating direction implicit (ADI) method. Here, the model problem is a partial differential equation system having two or more independent spatial coordinates. Its direct solution requires too much computer storage and time to be tractable. Using an ADI splitting, the problem is reduced to a manageable sequence of one-dimensional problems. In terms of the defect corrections, the system P is the sequence of one-dimensional problems that is much easier to solve, yet that closely approximates the original system.

Other forms of splitting also arise. For example, in certain systems of partial differential equations some of the equations are weakly coupled to the others. In these cases, solving the equations sequentially (rather than coupled) can result in significant savings. Similarly, in some combustion problems, considerable savings are realized through operator splitting algorithms in which the chemical rate terms are handled separately from the species transport terms. These methods are equivalent to matrix splittings of the Jacobian of the system.

Analysis of splitting methods is important because the methods often do not converge. We must be concerned about accuracy and convergence of the factored system. Even though each iteration may be fast, we must have some idea about the overall convergence rates and about any degradation in accuracy resulting from the split. Analysis will also likely lead to the identification of matrix properties that suggest a beneficial splitting that would not be apparent from physical reasoning. Splitting can be considered as either a splitting of the original equations or as an approximate factorization of the iteration matrix. The former is the most intuitive, and the one in which physical insight is valuable. However, the latter is probably the one more amenable to analysis.

4.8 MONTE CARLO TECHNIQUES

Mathematical solution methods can be broken into two broad classes, Monte Carlo methods and deterministic methods, depending on whether chance events are included in the method. All scientists are familiar with deterministic methods but most have little familiarity with Monte Carlo methods. Deterministic methods do not depend on chance, and calculations performed using the same input data and the same computer code will provide exactly the same results. Monte Carlo calculations using the same input data and the same computer code will provide different results, depending on what chance events occur. In this section we discuss what Monte Carlo methods are and how they might be improved.

The Monte Carlo method estimates averages on a probability model. Any quantity that can be expressed as an average value can be calculated by Monte Carlo techniques. Sometimes a probability model is obvious from the problem itself. For example, the probability that tossing three fair coins and obtaining a desired outcome [for example two heads (H) and one tail (T)] is easily estimated by Monte Carlo methods. The probability model consists of assigning a probability of $\frac{1}{2}$ to an H and a probability of $\frac{1}{2}$ to a T on each toss and assigning a score of 1 to a desired outcome (HHT, HTH, THH) and a score of 0 to any other outcome (HHH, TTT, THT, HTT, TTH). The computer has a random number generator that generates random numbers uniformly on the unit interval (0,1). A uniform distribution means that any random number ξ is equally likely to have any value between 0 and 1. Thus a coin toss can be simulated on a computer by:

H occurs if $\xi < \frac{1}{2}$
T occurs if $\xi > \frac{1}{2}$

To toss three coins the computer uses three random numbers ξ_1, ξ_2, and ξ_3. A typical set of tosses might be $\xi_1 = 0.7$ (T), $\xi_2 = 0.1$ (H), and $\xi_3 = 0.4$ (H), scoring 1. The probability of obtaining two heads and one tail is (approximately) the average score ($\frac{3}{8}$) after many sets of computer tosses.

Sometimes a probability model is not immediately apparent, but after a little thought the desired calculation can often be expressed as the estimation of an average value. For example, the integral

$$I = \frac{1}{b-a}\int_a^b f(x)dx$$

can be thought of as the average value of $f(x)$ on the interval (a, b). To see this, note that by definition the average value of $f(x)$ with respect to a probability density $p(x)$ is

$$<f> = \int_a^b f(x)p(x)dx.$$

Thus I is the average value of $f(x)$ with respect to the probability density $p(x) = 1/(b-a)$. Here $p(x)$ is a uniform probability density on (a, b), and

x values can be samples uniformly on (a, b) by setting

$$x_i = a + (b - a)\xi_i$$

whereupon

$$\hat{I} = \frac{1}{N}\sum_{i=l}^{N} f(x_i)$$

where $\hat{I}$ is the estimate of I.

There are many applications for the Monte Carlo technique, but the application to neutron and photon transport has probably consumed more computer time than all other applications combined. Because of this, and because neutron and photon transport problems have a natural probability model, the remaining discussion will pertain to neutron or photon transport problems. Furthermore, because neutron and photon transport are similar, the remaining discussion will refer to particle transport.

Particle flow in nature is a random process. One cannot say exactly what will happen to an individual particle. One can only say what the probabilities are that various events occur. For example, a particle traveling through matter has a certain probability to collide per unit distance; the actual distance between collisions is unknown, but the probability of traveling a distance l without collisions is known. Similarly the nuclide a particle will collide with is not known, but the probability of colliding with the nuclide is known.

The simplest Monte Carlo model for particle transport problems uses the natural probabilities that various events occur for the probability model in essentially the same way as the coin toss example. That is, particles are followed from event to event in a computer, and the next event is always selected (using the random number generator) from a number of possible next events according to the natural event probabilities. This type of model is called the analog Monte Carlo model because it is directly analogous to the naturally occurring transport.

The analog Monte Carlo model works well when a significant fraction of the particles contributes to the estimate of the average. This is analogous to having a significant fraction of the particles in the physical situation entering a detector. There are many problems for which the fraction of particles contribution (scoring) is very small, less than 10^{-6}. For these problems, analog Monte Carlo fails because few, if any, of the particles contribute, and the statistical uncertainty in the answer is unacceptable.

Although the analog Monte Carlo model is probably the simplest conceptual probability model, there are an infinite number of probability models for particle transport that will estimate the same average value as the analog Monte Carlo model. These other techniques are known as nonanalog Monte Carlo models, and they are useful because although the average value remains unchanged, the variance (uncertainty) of the estimate can often be made much smaller than the variance for the analog estimate. Practically this means that problems that would be impossible to solve in days of computer time can be solved in minutes of computer time.

A nonanalog Monte Carlo model attempts to follow "interesting" particles more often than noninteresting particles. An "interesting" particle, by definition, is a particle that contributes a large amount to the quantity (or quantities) that needs to be estimated. There are many nonanalog techniques, and they all are meant to increase the odds that a particle scores (contributes). To ensure that the average score is the same in the nonanalog game as in the analog game, the score is modified to remove the effect of biasing (changing) the natural odds. Thus, if a particle is artificially made q times as likely to execute a given random walk, then the particle's score is weighted by (that is, multiplied by) $1/q$. The average score is thus preserved because the average score is the sum, over all random walks, of the probability of a random walk and the score due to that random walk. The trick in obtaining low-variance solutions is to choose q's such that all random walks contribute the same score, in fact the average score. This then would be a zero-variance solution.

It is always possible for any (linear) particle transport problem to select q's for each random walk such that every particle's score is the average score; that is, a zero-variance solution. The hooker is, of course, that the perfect q's are not known, thus a zero-variance solution is not practical. However, people have often been successful enough in guessing good q's, that is biasing the odds, to improve the calculational efficiency by several orders of magnitude. This is typically done iteratively with a person making several short Monte Carlo computer runs (calculations) and using information gained on each run to better guess how to bias the next run. When the person's guesses no longer improve the calculation, a long run is done with the optimal biasing learned in the short runs.

Can the computer learn to optimize the biasing? The computer is, after all, supplying the information that the person uses to learn. In the past decade a number of computer learning techniques have been tested. Thus far it has proven impossible for a computer to take an arbitrary transport problem and, without human aid, optimize the biasing. However, two things are worthy of note. First, computer learning aided by human judgment appears to be substantially better in many cases than human learning alone. This typically works by having the computer inform the person how the computer would bias the subsequent run and having the person selectively alter the computer's suggestions according to the person's intuition. Second, the amount of human judgment required is decreasing. The day may come when the computer needs no human aid.

Once human aid is no longer needed, the computer can learn to adjust its own biasing particle, as the calculation proceeds. An interesting implication of an adaptive Monte Carlo technique is that the common central limit theorem of statistics that would constrain the accuracy of the calculation to decrease as the square root of the number of particles followed no longer applies. The common central limit theorem applies only when each particle's random walk is independent of all others and the sampling process is identical for all particles. Consequently, the rate of convergence may be more rapid. Although some limited statistical theories exist for dependent random variables, it has not been investigated whether these theories can profitably be applied to Monte Carlo particle transport problems. Thus, it is uncertain how fast an adaptive Monte Carlo calculation is converging or indeed what the maximum convergence rate for a good learning process might be. Empirical evidence shows that the convergence can be substantially faster than the square root of the number of particles. In light of this, Monte Carlo methods can be expected to become more competitive with deterministic calculations.

4.9 PROBLEM-DEPENDENT METHODS

A variety of adaptive methods have a common goal: to overcome the computer size and grid resolution limitations, which are especially severe in singular problems, by use of computational elements that fit or model the singularity more directly. In this way, it may be possible to incorporate into the solution algorithm considerable analytic information beyond that provided by the equations themselves. This theme occurs in many aspects of numerical analysis. In the finite-element method, one may choose elements that include any singularities in the solution being computed (see Section 3.3). Grid adaptivity (see Section 4.2) is also problem dependent. Here we discuss examples of somewhat more special methods. Of necessity they apply only to classes of problems that possess related singularities.

4.9.1 The Riemann Problem and Nonlinear Wave Modes

The Riemann problem for a nonlinear hyperbolic system of conservation laws is the Cauchy problem in one space dimension for data that are everywhere constant except for a single jump discontinuity at the origin. The solution of the Riemann problem provides a resolution of this discontinuity into the nonlinear modes, or waves, which propagate coherently in time. This idealized problem can be thought of as an approximate description of a higher-dimensional flow field especially in the neighborhood of a discontinuity hypersurface. This point of view has led to a number of improved finite-difference schemes, which attempt to determine the various nonlinear wave modes at each point in space and time and to adjust the differencing of the differential equations to take advantage of this knowledge. This adaptivity is to the structure of state space, in contrast to the coordinate space adaptivity discussed in Section 4.2.

4.9.2 Front Tracking

Front tracking is a combination of adaptive grid methods with the use of Riemann problems. The method is adapted to problems that have important singularity hypersurfaces (lines in two space dimensions, surfaces in three space dimensions), such as shock waves and contact discontinuities. In one version of this method, there is an overall time-dependent coordinate transformation to map the discontinuity into a fixed grid line in some set of computational coordinates. In another version, the discontinuity is represented by a moving lower-dimensional grid that follows ("tracks") the dynamical motion of the discontinuity. The motion of the discontinuity and of the moving grid points that track it are governed by solutions of Riemann problems, or equivalently by the method of characteristics.

4.9.3 Vortex Method

This method introduces small lines or surfaces of vorticity into a fluid flow. The method is adapted to the study of shear-layer discontinuities, boundary layers, boundary-layer separation, and turbulence. The equations of motion of an ideal fluid yield simple equations for the motion of a collection of vortices imbedded in the fluid. In fact, the vortices move passively with the fluid, and their mutual interaction is described by a Hamiltonian system of ordinary differential equations, with Coulomb type interaction energy. In the case of the Navier-Stokes equations, the vortex motion also contains a diffusion term.

These methods have been applied successfully to the problem of turbulent flame propagation (see Section 2.2). In this problem, the turbulent mixing is a primary factor in determining the flame speed. The turbulence comes from the boundary layer and in the boundary layer is calculated by a vortex method. Related methods have been developed under a variety of names such as boundary integral methods and Green's function methods.

4.9.4 Scale Invariance and the Renormalization Group

Scale transformations are the transformations $x \to sx$, acting on space or on space and time. A function u is homogeneous of degree α if

$$u(sx, sy, sz) = s^{\alpha} u(x, y, z)$$

and scale invariant if $\alpha = 0$. Many problems have solutions that are scale invariant or approximately scale invariant over some parameter range. Such solutions are called similarity solutions. Using the scale invariance, one of the independent variables can be eliminated, making the solution more elementary to compute.

However, scale invariance can also indicate the occurrence of complex phenomena. Specifically, any singularity that occurs in a scale-invariant problem must be repeated in all length scales (for which the scale invariance holds). Mathematically, Cantor sets, snowflake curves, and fractals are examples of such phenomena. In statistical physics, critical phenomena in the equation of state is a scale-invariant problem. One general picture of turbulence holds that scale invariance (vortices on a large range of length scales) describe the inertial range, or energy transport range, of turbulence.

To implement these ideas in a computational algorithm, one integrates over a given set of length scales in a standard manner. The result of this computation is taken as data for a new calculation over a new set of length scales (with the original degrees of freedom eliminated from the problem). This process is iterated and if convergent gives the scale exponent α. Sample numerical calculations of this type were discussed in Section 2.1 in connection with turbulence. The method is well established for perturbative calculations (with a small parameter) in critical phenomena in statistical physics.

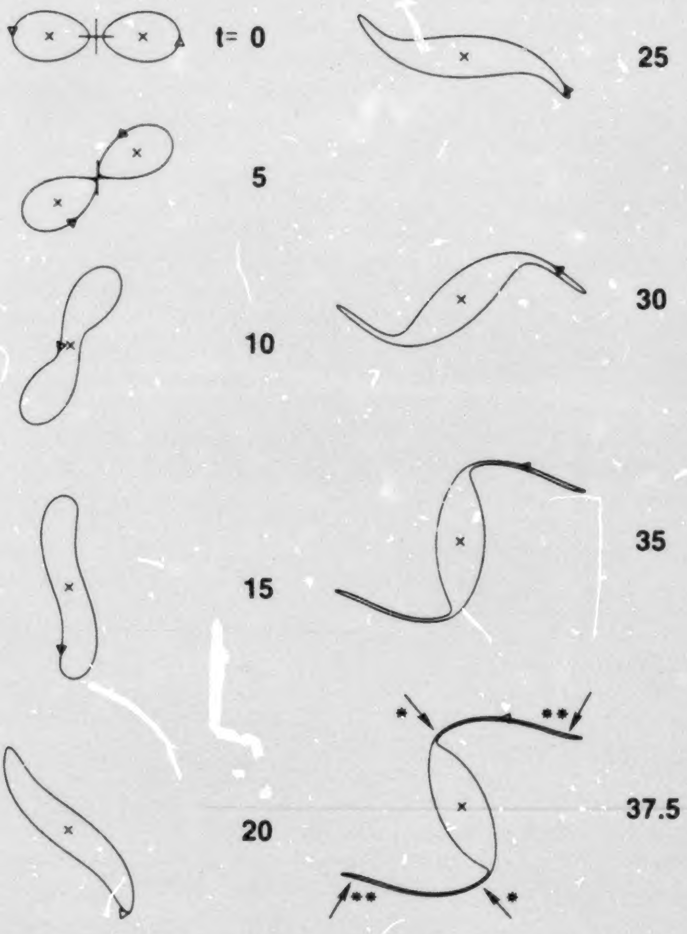


FIGURE 4.1 The evolution and merger of isolated vortex structures as predicted by contour dynamical techniques. [From E. A. Overman II and N. J. Zabusky, *Phys. Fluids* **25**, 1297-1305 (1982).]

Since the renormalization group methods are novel, it is worth mentioning that the mathematical foundations of this method have been established recently in several cases including examples of hierarchical models in statistical mechanics, interval maps, and renormalized quantum fields.

4.9.5 Contour Dynamical Methods

Contour dynamical methods are being applied to a variety of incompressible flows in two dimensions. These generalizations of the "waterbag" method provide simplified models for following the evolution of contours separating regions of piecewise-constant (pc) density that are the sources of the flow. The flow is the result of the self and mutual interaction of contours that evolve, mainly by area-preserving maps. These methods have been applied to the Euler equations, where pc finite-area-vortex regions and/or vortex sheets at density interfaces are sources of the flow; and the equations for a weakly ionized and strongly magnetized ionospheric plasma cloud, where pc ion-density regions are sources of the flow. For the former, a large class of steady-state translating and rotating solutions with pc vorticity ("V-states") have been found. Figure 4.1 shows the merger and breaking for a perturbed corotating V-state (two pc finite-area vortex regions with the same circulation), a familiar process in free-shear layer experiments. Notice how the two regions merge to form one region (by snipping out the common boundary at $t = 10$) and then stabilize by ejecting vorticity in thin filaments. With these methods it is possible to obtain detailed information about the regions because the dimension is reduced by one. The curvature of the contour provides a predictive signature of the evolving small-scale structure, e.g., the roll up of vorticity filaments, etc.

4.10 COMPUTER SOFTWARE AND HARDWARE

As previously discussed, large-scale scientific calculations that tax the resources of the most powerful computers will continue to be essential to modern research and development efforts. To obtain long-term reliability and stability of future applications codes, implementing and testing of high-level numerical software should be coordinated. This will require a strong research and development effort with cooperation supported among applications programmers, the theoretical numerical methods researchers, and the computer-science software developers.

Repetition of expensive, error-prone, and time-consuming coding of commonly used methods should be avoided. Much of the current scientific software now being developed is redundant. If the common elements of the existing codes were available as modules, future applications programmers could use these routines and eliminate much of their efforts. New software is most readily accepted if it is compatible with existing techniques and simple enough so that potential users can observe tangibly better results in a trial run than those existing methods can produce. If such high-level routines were available, they could perform many of the common procedures found in applications codes, including grid generation, rezoning, numerical interpolation, differentiation, and integration; they could approximate differential boundary conditions and solve large, sparse nonlinear systems of equations.

An important goal is the machine independence of applications programs. This is a difficult task because methods tailored specifically for a particular machine architecture will probably become more the norm than the exception. We can, by keeping machine-dependent codes in libraries of high-level software with standard user interfaces, strive to keep the user's scientific applications codes portable. The underlying library routines will be, necessarily, less portable because the architecture of the new machines will certainly be different from that of today's supercomputers. To utilize the inherent powers of the new machines we will have to re-examine traditional methods and identify the better ones for a particular machine architecture.

The continuing revolution in microelectronics is having a profound impact on scientific computing. Indeed, it is likely to change our concept dramatically of what scientific computations can and cannot be effectively performed. Most certainly the impact of this revolution will be much greater than, say, the impact that floating-point hardware had. Moreover, while the costs of individual tasks will be greatly reduced, the domain of scientific computations will be greatly expanded and "frontier computations" will continue to be expensive.

These changes are being brought about by a number of factors: Individual components are becoming increasingly faster and smaller. Very-large-scale integration of such components is not only reducing the size of the packaged systems but also providing opportunities for customized information processors. Also, the decrease in the cost and size of computer memory implies that we can look for much larger memory systems. This will obviate many of the existing difficulties with secondary storage.

Despite the fact that components are becoming faster, the limits of raw machine speed are not visible, and further gains will eventually have to be made by using clever architectures and algorithms. Some kind of parallelism seems to be unavoidable. The programming issues involved in using parallel machines are still not satisfactorily resolved. The automatic detection of parallelism and the resulting scheduling of multiple resources are important open problems.

Architectures, such as systolic arrays, based on specific subtasks can increase the performance of systems involving these subtasks by several orders of magnitude and clearly have a bright future. Algorithms containing compute-intensive subtasks that can be vectorized in this fashion have a bright future. Because these architectures are in general regular, the algorithms that can be vectorized for such machines tend to be regular, i.e., simple, nonadaptive, uniform-grid, low-order algorithms. It is clear that there are nicely behaved problems for which these regular algorithms on specialized machines will require significantly less time than algorithms requiring fewer operations on serial machines. It is also clear that no matter how fast the specialized machines are, there are problems that are sufficiently difficult that more sophisticated algorithms are needed for more general-purpose computers.

In order to bring about these advances in architecture, it is necessary to involve practitioners of scientific computation in the design process. Luckily, modern design automation tools should make it possible for interdisciplinary design teams to successfully synthesize innovative special-purpose systems, and automated fabrication facilities should make it possible for such systems to be built, debugged, and used.

These advances in machine architecture should also have a dramatic effect on the design and analysis of algorithms for scientific computing. Traditionally, such analysis has been based on (asymptotic) estimates of the number of arithmetic operations. However, with these new architectures it is quite likely that the running time of an algorithm will be more dependent on the movement of data than on the number of arithmetic operations. Thus, we need to develop new analytic models of complexity of scientific algorithms so that such models give us useful information about the relative performance of algorithms.

Appendix A
Persons Contributing to this Report

Ivo Babŭska, University of Maryland
K. Binder, KFA Julich GmbH, Institut Festkorperforschung
Norman Bleistein, University of Denver
Thomas E. Booth, Los Alamos National Laboratory
Billy L. Buzbee, Los Alamos National Laboratory
William S. Childress, New York University
Alexandre J. Chorin, University of California, Berkeley
Lawrence D. Cloutman, Los Alamos National Laboratory
James P. Corones, Ames Laboratory, Iowa State University
Joel E. Dendy, Los Alamos National Laboratory
Paul P. Eggermont, University of Delaware
Alan J. Faller, University of Maryland
Paul R. Garabedian, New York University
John M. Greene, General Atomics Company
Eugene Isaacson, New York University
Jasper A. Jackson, Los Alamos National Laboratory
Malvin H. Kalos, New York University
Herbert B. Keller, California Institute of Technology
Heins-Otto Kreiss, California Institute of Technology
Edward W. Larsen, Los Alamos National Laboratory
Peter D. Lax, New York University
Joel Lebowitz, Rutgers University
Dennis R. Liles, Los Alamos National Laboratory
C. C. Lin, Massachusetts Institute of Technology
Oscar Manley, U. S. Department of Energy
Steven B. Margolis, Sandia National Laboratories
Jerrold E. Marsden, University of California, Berkeley
Oliver A. McBryan, New York University
Keith Miller, University of California, Berkeley
Cathleen S. Morawetz, New York University
M. Zahair Nashed, University of Delaware
J. Tinsley Oden, University of Texas
Edward A. Overman II, University of Pittsburgh
Edward Ott, University of Maryland

George C. Papanicolaou, New York University
Charles S. Peskin, New York University
Linda R. Petzold, Sandia National Laboratories
Thomas F. Porsching, University of Pittsburgh
Garry H. Rodrigue, Lawrence Livermore National Laboratory
Jacob T. Schwartz, New York University
Philip E. Seiden, IBM Corporation
David H. Sharp, Lawrence Livermore National Laboratory
Lawrence A. Shepp, Bell Laboratories
Mitchell D. Smooke, Sandia National Laboratories
Blair K. Swartz, Los Alamos National Laboratory
Yvain M. Treve, La Jolla Institute
Michael Steenstrup Vogelius, University of Maryland
Burton Wendroff, Los Alamos National Laboratory
Norman J. Zabusky, University of Pittsburgh

National Academy Press

The National Academy Press was created by the National Academy of Sciences to publish the reports issued by the Academy and by the National Academy of Engineering, the Institute of Medicine, and the National Research Council, all operating under the charter granted to the National Academy of Sciences by the Congress of the United States.

BEST COPY AVAILABLE